



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 12, 2026 – 04:16 PM UTC

PDB ID : 2MVD / pdb\_00002mvd  
BMRB ID : 25261  
Title : Solution structure of [GlnB22]-insulin mutant at pH 1.9  
Authors : Hexnerova, R.; Krizkova, K.; Maletinska, L.; Jiracek, J.; Brzozowski, A.M.;  
Zakova, L.; Veverka, V.  
Deposited on : 2014-10-02

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

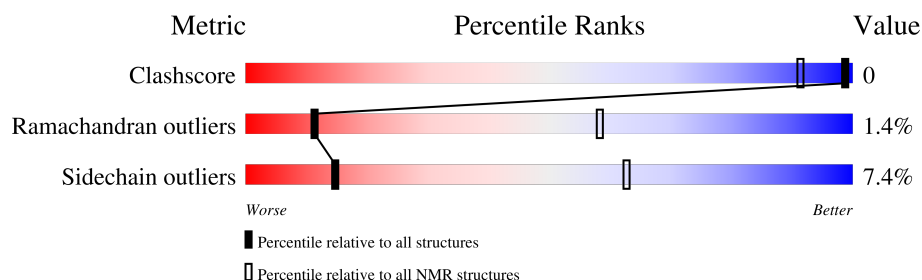
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 51%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 21     | <br>95% 5%       |
| 2   | B     | 30     | <br>80% 20%      |

## 2 Ensemble composition and analysis

This entry contains 40 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

| Well-defined (core) protein residues |                          |                   |              |
|--------------------------------------|--------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)    | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:1-A:21, B:31-B:54 (45) | 1.30              | 16           |

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 5 clusters and 3 single-model clusters were found.

| Cluster number        | Models                                                                                                  |
|-----------------------|---------------------------------------------------------------------------------------------------------|
| 1                     | 1, 2, 3, 4, 6, 8, 9, 10, 12, 13, 14, 15, 16, 17, 18, 20, 21, 22, 23, 24, 26, 27, 30, 31, 32, 34, 37, 40 |
| 2                     | 25, 33, 38                                                                                              |
| 3                     | 11, 39                                                                                                  |
| 4                     | 5, 28                                                                                                   |
| 5                     | 7, 35                                                                                                   |
| Single-model clusters | 19; 29; 36                                                                                              |

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 785 atoms, of which 382 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Insulin A chain.

| Mol | Chain | Residues | Atoms |    |     |    |    |   | Trace |
|-----|-------|----------|-------|----|-----|----|----|---|-------|
| 1   | A     | 21       | Total | C  | H   | N  | O  | S | 0     |
|     |       |          | 314   | 99 | 151 | 25 | 35 | 4 |       |

- Molecule 2 is a protein called Insulin B chain.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 2   | B     | 30       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 471   | 157 | 231 | 38 | 43 | 2 |       |

There is a discrepancy between the modelled and reference sequences:

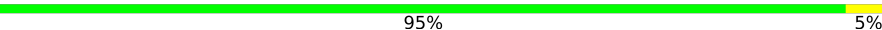
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | 52      | GLN      | ARG    | engineered mutation | UNP P01308 |

## 4 Residue-property plots

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

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

- Molecule 1: Insulin A chain

Chain A: 



- Molecule 2: Insulin B chain

Chain B: 



### 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: Insulin A chain

Chain A: 



- Molecule 2: Insulin B chain

Chain B: 



### 4.2.2 Score per residue for model 2

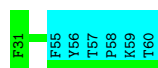
- Molecule 1: Insulin A chain

Chain A:  90% 10%



- Molecule 2: Insulin B chain

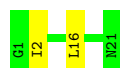
Chain B:  80% 20%



### 4.2.3 Score per residue for model 3

- Molecule 1: Insulin A chain

Chain A:  90% 10%



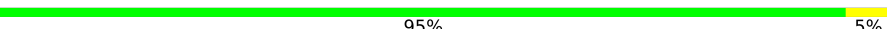
- Molecule 2: Insulin B chain

Chain B:  73% 7% 20%



### 4.2.4 Score per residue for model 4

- Molecule 1: Insulin A chain

Chain A:  95% 5%



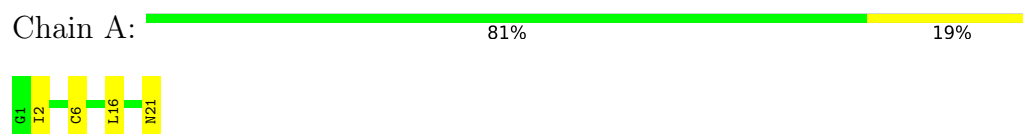
- Molecule 2: Insulin B chain

Chain B:  70% 10% 20%

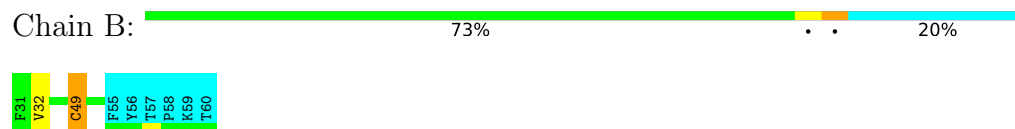


#### 4.2.5 Score per residue for model 5

- Molecule 1: Insulin A chain

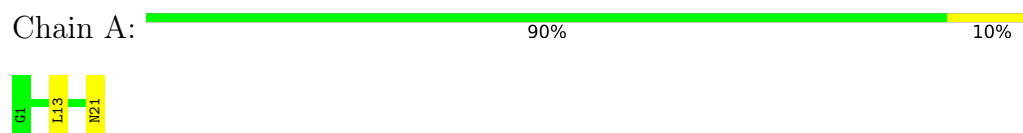


- Molecule 2: Insulin B chain

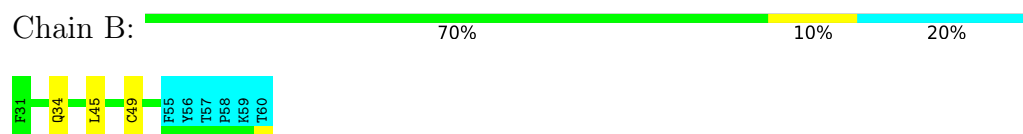


#### 4.2.6 Score per residue for model 6

- Molecule 1: Insulin A chain

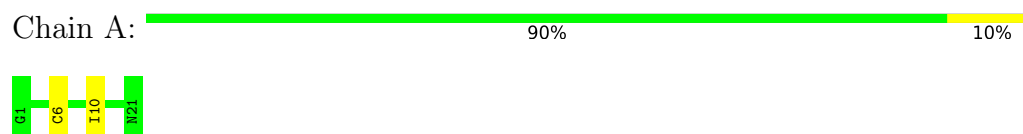


- Molecule 2: Insulin B chain

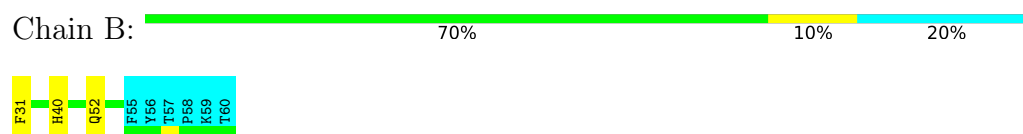


#### 4.2.7 Score per residue for model 7

- Molecule 1: Insulin A chain



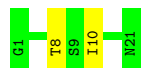
- Molecule 2: Insulin B chain



### 4.2.8 Score per residue for model 8

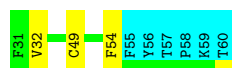
- Molecule 1: Insulin A chain

Chain A:  90% 10%



- Molecule 2: Insulin B chain

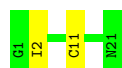
Chain B:  70% 10% 20%



### 4.2.9 Score per residue for model 9

- Molecule 1: Insulin A chain

Chain A:  90% 10%



- Molecule 2: Insulin B chain

Chain B:  77% 20%



### 4.2.10 Score per residue for model 10

- Molecule 1: Insulin A chain

Chain A:  90% 5% 5%



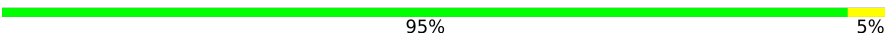
- Molecule 2: Insulin B chain

Chain B:  77% 20%



#### 4.2.11 Score per residue for model 11

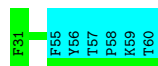
- Molecule 1: Insulin A chain

Chain A:  95% 5%



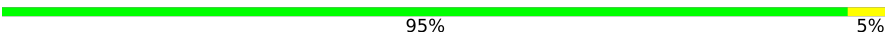
- Molecule 2: Insulin B chain

Chain B:  80% 20%



#### 4.2.12 Score per residue for model 12

- Molecule 1: Insulin A chain

Chain A:  95% 5%



- Molecule 2: Insulin B chain

Chain B:  73% 7% 20%



#### 4.2.13 Score per residue for model 13

- Molecule 1: Insulin A chain

Chain A:  81% 19%



- Molecule 2: Insulin B chain

Chain B:  73% 7% 20%



#### 4.2.14 Score per residue for model 14

- Molecule 1: Insulin A chain

Chain A:  90% 10%



- Molecule 2: Insulin B chain

Chain B:  73% 7% 20%



#### 4.2.15 Score per residue for model 15

- Molecule 1: Insulin A chain

Chain A:  90% 10%



- Molecule 2: Insulin B chain

Chain B:  73% 7% 20%



#### 4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Insulin A chain

Chain A:  86% 14%



- Molecule 2: Insulin B chain

Chain B:  73% 7% 20%



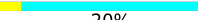
#### 4.2.17 Score per residue for model 17

- Molecule 1: Insulin A chain

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Insulin B chain

Chain B:  77%  20%



#### 4.2.18 Score per residue for model 18

- Molecule 1: Insulin A chain

Chain A:  76%  24%



- Molecule 2: Insulin B chain

Chain B:  73%  7%  20%



#### 4.2.19 Score per residue for model 19

- Molecule 1: Insulin A chain

Chain A:  95%  5%



- Molecule 2: Insulin B chain

Chain B:  67%  13%  20%



#### 4.2.20 Score per residue for model 20

- Molecule 1: Insulin A chain

Chain A:  90% 10%



- Molecule 2: Insulin B chain

Chain B:  77% 20%



#### 4.2.21 Score per residue for model 21

- Molecule 1: Insulin A chain

Chain A:  95% 5%



- Molecule 2: Insulin B chain

Chain B:  77% 20%



#### 4.2.22 Score per residue for model 22

- Molecule 1: Insulin A chain

Chain A:  81% 19%



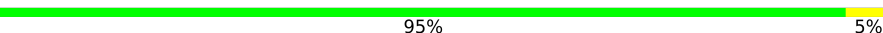
- Molecule 2: Insulin B chain

Chain B:  73% 7% 20%



#### 4.2.23 Score per residue for model 23

- Molecule 1: Insulin A chain

Chain A:  95% 5%



- Molecule 2: Insulin B chain

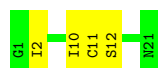
Chain B:  70% 10% 20%



#### 4.2.24 Score per residue for model 24

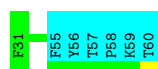
- Molecule 1: Insulin A chain

Chain A:  81% 19%



- Molecule 2: Insulin B chain

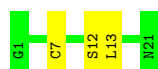
Chain B:  80% 20%



#### 4.2.25 Score per residue for model 25

- Molecule 1: Insulin A chain

Chain A:  86% 14%



- Molecule 2: Insulin B chain

Chain B:  73% 7% 20%



#### 4.2.26 Score per residue for model 26

- Molecule 1: Insulin A chain

Chain A:  86% 14%



- Molecule 2: Insulin B chain

Chain B:  67% 13% 20%



#### 4.2.27 Score per residue for model 27

- Molecule 1: Insulin A chain

Chain A:  86% 14%



- Molecule 2: Insulin B chain

Chain B:  77% • 20%



#### 4.2.28 Score per residue for model 28

- Molecule 1: Insulin A chain

Chain A:  95% 5%



- Molecule 2: Insulin B chain

Chain B:  77% • 20%



#### 4.2.29 Score per residue for model 29

- Molecule 1: Insulin A chain

Chain A:  81% 19%



- Molecule 2: Insulin B chain

Chain B:  73% 20%



#### 4.2.30 Score per residue for model 30

- Molecule 1: Insulin A chain

Chain A:  86% 10% 5%



- Molecule 2: Insulin B chain

Chain B:  77% 20%



#### 4.2.31 Score per residue for model 31

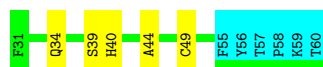
- Molecule 1: Insulin A chain

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Insulin B chain

Chain B:  63% 17% 20%



### 4.2.32 Score per residue for model 32

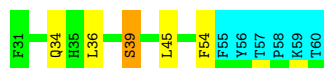
- Molecule 1: Insulin A chain

Chain A:  90% 10%



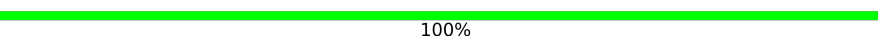
- Molecule 2: Insulin B chain

Chain B:  63% 13% 20%



### 4.2.33 Score per residue for model 33

- Molecule 1: Insulin A chain

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Insulin B chain

Chain B:  73% 7% 20%



### 4.2.34 Score per residue for model 34

- Molecule 1: Insulin A chain

Chain A:  86% 14%



- Molecule 2: Insulin B chain

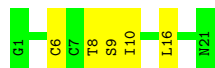
Chain B:  73% 7% 20%



#### 4.2.35 Score per residue for model 35

- Molecule 1: Insulin A chain

Chain A:  76% 24%



- Molecule 2: Insulin B chain

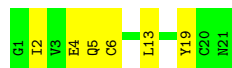
Chain B:  77% 20%



#### 4.2.36 Score per residue for model 36

- Molecule 1: Insulin A chain

Chain A:  71% 29%



- Molecule 2: Insulin B chain

Chain B:  60% 20% 20%



#### 4.2.37 Score per residue for model 37

- Molecule 1: Insulin A chain

Chain A:  95% 5%



- Molecule 2: Insulin B chain

Chain B:  70% 7% 20%



#### 4.2.38 Score per residue for model 38

- Molecule 1: Insulin A chain

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Insulin B chain

Chain B:  77% 20%



#### 4.2.39 Score per residue for model 39

- Molecule 1: Insulin A chain

Chain A:  86% 14%



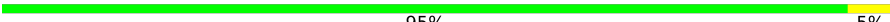
- Molecule 2: Insulin B chain

Chain B:  77% 20%



#### 4.2.40 Score per residue for model 40

- Molecule 1: Insulin A chain

Chain A:  95% 5%



- Molecule 2: Insulin B chain

Chain B:  63% 17% 20%



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 40 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution |         |
| YASARA        | refinement         |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 344            |
| Number of shifts mapped to atoms             | 344            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 51%            |

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 1.35±0.17    | 0±1/164 ( 0.3± 0.4%) | 1.10±0.12   | 0±0/220 ( 0.1± 0.2%) |
| 2   | B     | 1.30±0.18    | 0±0/191 ( 0.1± 0.2%) | 1.05±0.09   | 0±0/259 ( 0.0± 0.1%) |
| All | All   | 1.33         | 26/14200 ( 0.2%)     | 1.08        | 10/19160 ( 0.1%)     |

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

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 2   | ILE  | CA-CB | 10.46 | 1.66        | 1.54     | 24     | 9     |
| 2   | B     | 42  | VAL  | CA-CB | 7.83  | 1.64        | 1.54     | 13     | 1     |
| 2   | B     | 32  | VAL  | CA-CB | 7.16  | 1.63        | 1.54     | 29     | 2     |
| 1   | A     | 1   | GLY  | N-CA  | 6.19  | 1.55        | 1.45     | 32     | 1     |
| 2   | B     | 49  | CYS  | CA-C  | 6.05  | 1.60        | 1.52     | 29     | 1     |
| 1   | A     | 10  | ILE  | CA-CB | 6.04  | 1.61        | 1.54     | 40     | 7     |
| 1   | A     | 21  | ASN  | C-OXT | 6.03  | 1.35        | 1.23     | 6      | 1     |
| 2   | B     | 44  | ALA  | CA-CB | 5.71  | 1.62        | 1.53     | 31     | 1     |
| 2   | B     | 47  | LEU  | C-O   | -5.26 | 1.17        | 1.24     | 14     | 1     |
| 2   | B     | 39  | SER  | N-CA  | 5.07  | 1.52        | 1.46     | 32     | 1     |
| 1   | A     | 4   | GLU  | C-O   | -5.02 | 1.17        | 1.24     | 36     | 1     |

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

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|----------|-------|-------------|----------|--------|-------|
|     |       |     |      |          |       |             |          | Worst  | Total |
| 2   | B     | 52  | GLN  | N-CA-C   | -6.91 | 103.83      | 111.36   | 15     | 2     |
| 1   | A     | 21  | ASN  | CA-CB-CG | -5.40 | 107.20      | 112.60   | 29     | 2     |
| 1   | A     | 19  | TYR  | N-CA-C   | -5.39 | 106.20      | 112.89   | 36     | 1     |
| 2   | B     | 38  | GLY  | N-CA-C   | 5.38  | 115.11      | 110.21   | 22     | 1     |
| 1   | A     | 2   | ILE  | N-CA-C   | 5.33  | 115.95      | 110.36   | 37     | 2     |
| 2   | B     | 34  | GLN  | N-CA-C   | -5.25 | 100.94      | 108.60   | 6      | 1     |
| 2   | B     | 31  | PHE  | CA-CB-CG | 5.07  | 118.87      | 113.80   | 7      | 1     |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 163   | 151      | 149      | 0±0     |
| 2   | B     | 186   | 178      | 172      | 0±0     |
| All | All   | 13960 | 13160    | 12840    | 4       |

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:2:ILE:HD12  | 1:A:19:TYR:CD2 | 0.52     | 2.39        | 1      | 2     |
| 1:A:2:ILE:HD12  | 1:A:19:TYR:CD1 | 0.43     | 2.48        | 10     | 1     |
| 1:A:13:LEU:HD21 | 2:B:31:PHE:CZ  | 0.42     | 2.50        | 19     | 1     |

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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

| Mol | Chain | Analysed        | Favoured     | Allowed     | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|-------------|------------|-------------|----|
| 1   | A     | 19/21 (90%)     | 18±1 (94±6%) | 1±1 (5±5%)  | 0±0 (1±2%) | 16          | 66 |
| 2   | B     | 23/30 (77%)     | 20±2 (88±8%) | 2±2 (10±7%) | 0±1 (2±3%) | 9           | 52 |
| All | All   | 1680/2040 (82%) | 1526 (91%)   | 130 (8%)    | 24 (1%)    | 11          | 58 |

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 54  | PHE  | 6              |
| 1   | A     | 10  | ILE  | 6              |
| 2   | B     | 38  | GLY  | 3              |
| 2   | B     | 36  | LEU  | 2              |
| 2   | B     | 49  | CYS  | 2              |
| 2   | B     | 52  | GLN  | 1              |
| 1   | A     | 11  | CYS  | 1              |
| 2   | B     | 39  | SER  | 1              |
| 2   | B     | 51  | GLU  | 1              |
| 2   | B     | 50  | GLY  | 1              |

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

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

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|-------------|----|
| 1   | A     | 20/20 (100%)    | 19±1 (93±6%) | 1±1 (7±6%) | 16          | 64 |
| 2   | B     | 20/26 (77%)     | 18±1 (92±6%) | 2±1 (8±6%) | 13          | 61 |
| All | All   | 1600/1840 (87%) | 1481 (93%)   | 119 (7%)   | 15          | 63 |

All 27 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) |
|-----|-------|-----|------|----------------|
| 2   | B     | 49  | CYS  | 11             |
| 1   | A     | 6   | CYS  | 10             |
| 2   | B     | 51  | GLU  | 8              |
| 1   | A     | 16  | LEU  | 8              |
| 2   | B     | 45  | LEU  | 8              |
| 1   | A     | 13  | LEU  | 8              |
| 2   | B     | 40  | HIS  | 8              |
| 1   | A     | 12  | SER  | 6              |
| 1   | A     | 2   | ILE  | 6              |
| 2   | B     | 37  | CYS  | 5              |
| 2   | B     | 32  | VAL  | 5              |
| 2   | B     | 39  | SER  | 4              |
| 2   | B     | 54  | PHE  | 4              |
| 1   | A     | 15  | GLN  | 4              |
| 2   | B     | 43  | GLU  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 8   | THR  | 3              |
| 2   | B     | 36  | LEU  | 3              |
| 1   | A     | 11  | CYS  | 3              |
| 1   | A     | 20  | CYS  | 2              |
| 2   | B     | 34  | GLN  | 2              |
| 1   | A     | 21  | ASN  | 1              |
| 1   | A     | 3   | VAL  | 1              |
| 1   | A     | 18  | ASN  | 1              |
| 1   | A     | 7   | CYS  | 1              |
| 1   | A     | 9   | SER  | 1              |
| 1   | A     | 5   | GLN  | 1              |
| 2   | B     | 42  | VAL  | 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 51% for the well-defined parts and 51% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 344 |
| Number of shifts mapped to atoms        | 344 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

#### 7.1.2 Chemical shift referencing

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

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 51%, i.e. 298 atoms were assigned a chemical shift out of a possible 583. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 89/229 (39%)  | 89/94 (95%)    | 0/90 (0%)       | 0/45 (0%)       |
| Sidechain | 184/291 (63%) | 184/191 (96%)  | 0/93 (0%)       | 0/7 (0%)        |
| Aromatic  | 25/63 (40%)   | 25/30 (83%)    | 0/29 (0%)       | 0/4 (0%)        |
| Overall   | 298/583 (51%) | 298/315 (95%)  | 0/212 (0%)      | 0/56 (0%)       |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 51%, i.e. 344 atoms were assigned a chemical shift out of a possible 670. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 100/257 (39%) | 100/105 (95%)  | 0/102 (0%)      | 0/50 (0%)       |
| Sidechain | 210/331 (63%) | 210/217 (97%)  | 0/106 (0%)      | 0/8 (0%)        |
| Aromatic  | 34/82 (41%)   | 34/39 (87%)    | 0/39 (0%)       | 0/4 (0%)        |
| Overall   | 344/670 (51%) | 344/361 (95%)  | 0/247 (0%)      | 0/62 (0%)       |

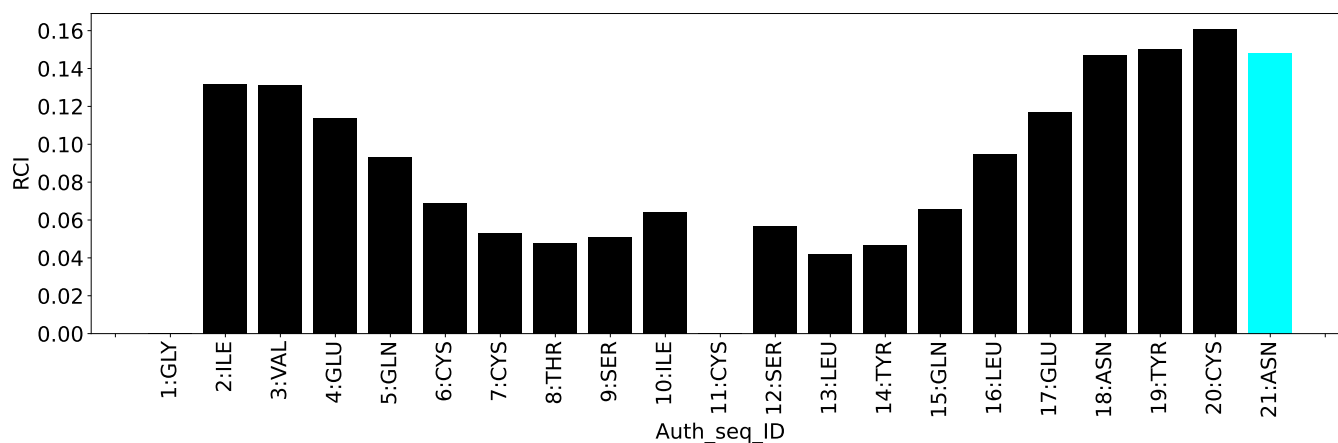
### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

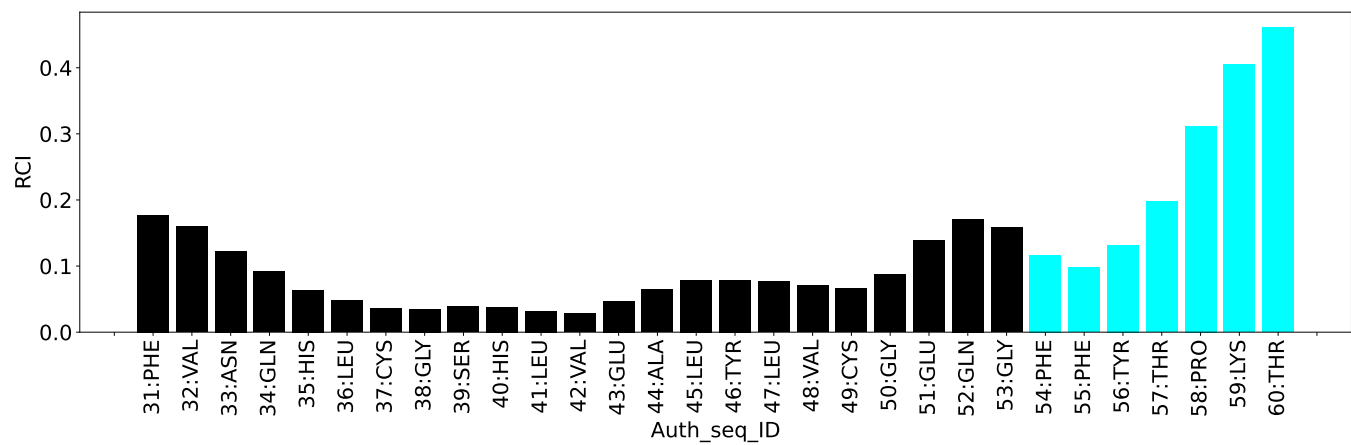
### 7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



## 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                                | 646   |
| Intra-residue ( $ i-j =0$ )                              | 178   |
| Sequential ( $ i-j =1$ )                                 | 156   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 129   |
| Long range ( $ i-j \geq 5$ )                             | 55    |
| Inter-chain                                              | 74    |
| Hydrogen bond restraints                                 | 48    |
| Disulfide bond restraints                                | 6     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 12.7  |
| Number of long range restraints per residue <sup>1</sup> | 1.1   |

<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)  | 8.8                                    | 0.2     |
| 0.2-0.5 (Medium) | 4.7                                    | 0.5     |
| >0.5 (Large)     | None                                   | None    |

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

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

## 9 Distance violation analysis ⓘ

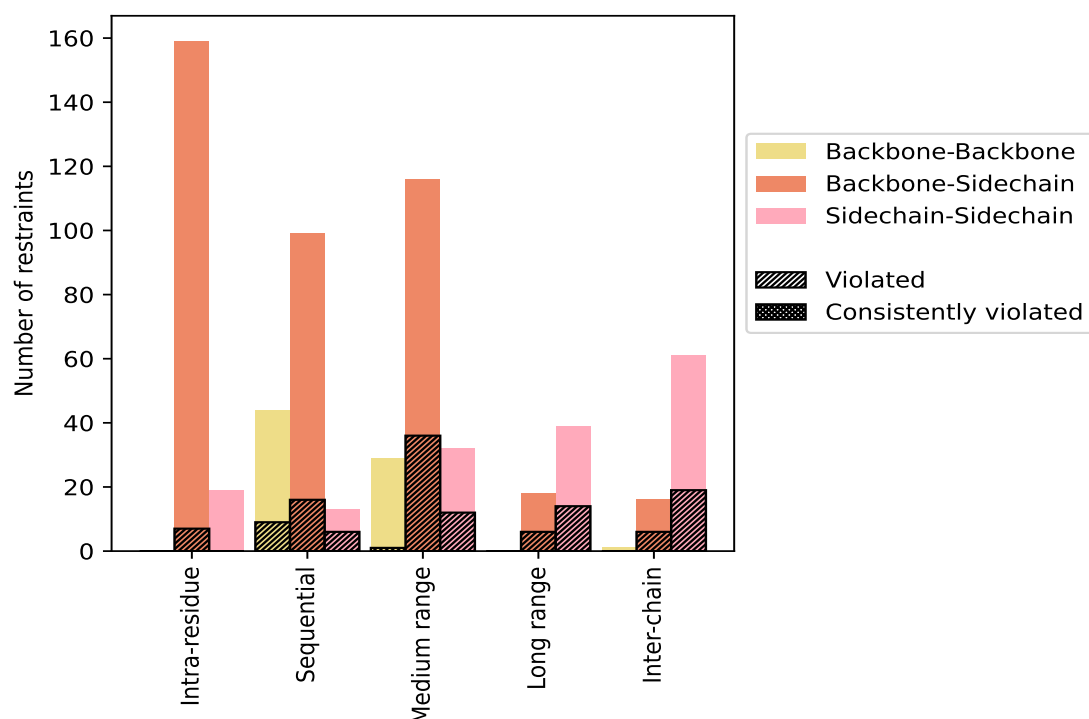
### 9.1 Summary of distance violations ⓘ

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

| 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>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">178</a> | <a href="#">27.6</a>  | <a href="#">7</a>     | <a href="#">3.9</a>  | <a href="#">1.1</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 159                 | 24.6                  | 7                     | 4.4                  | 1.1                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 19                  | 2.9                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">156</a> | <a href="#">24.1</a>  | <a href="#">31</a>    | <a href="#">19.9</a> | <a href="#">4.8</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 44                  | 6.8                   | 9                     | 20.5                 | 1.4                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 99                  | 15.3                  | 16                    | 16.2                 | 2.5                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 13                  | 2.0                   | 6                     | 46.2                 | 0.9                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">129</a> | <a href="#">20.0</a>  | <a href="#">27</a>    | <a href="#">20.9</a> | <a href="#">4.2</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 29                  | 4.5                   | 1                     | 3.4                  | 0.2                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 68                  | 10.5                  | 14                    | 20.6                 | 2.2                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 32                  | 5.0                   | 12                    | 37.5                 | 1.9                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">55</a>  | <a href="#">8.5</a>   | <a href="#">20</a>    | <a href="#">36.4</a> | <a href="#">3.1</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 18                  | 2.8                   | 6                     | 33.3                 | 0.9                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 37                  | 5.7                   | 14                    | 37.8                 | 2.2                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Inter-chain</a>                                | <a href="#">74</a>  | <a href="#">11.5</a>  | <a href="#">25</a>    | <a href="#">33.8</a> | <a href="#">3.9</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 1                   | 0.2                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 16                  | 2.5                   | 6                     | 37.5                 | 0.9                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 57                  | 8.8                   | 19                    | 33.3                 | 2.9                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">48</a>  | <a href="#">7.4</a>   | <a href="#">22</a>    | <a href="#">45.8</a> | <a href="#">3.4</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">6</a>   | <a href="#">0.9</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">646</a> | <a href="#">100.0</a> | <a href="#">132</a>   | <a href="#">20.4</a> | <a href="#">20.4</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 74                  | 11.5                  | 10                    | 13.5                 | 1.5                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 408                 | 63.2                  | 71                    | 17.4                 | 11.0                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 164                 | 25.4                  | 51                    | 31.1                 | 7.9                  | 0                                  | 0.0                 | 0.0                 |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 0                    | 2               | 4               | 1               | 2               | 9     | 0.16     | 0.27    | 0.05                | 0.14       |
| 2        | 0                    | 2               | 2               | 2               | 2               | 8     | 0.2      | 0.49    | 0.12                | 0.14       |
| 3        | 0                    | 1               | 1               | 1               | 2               | 5     | 0.3      | 0.49    | 0.11                | 0.23       |
| 4        | 0                    | 1               | 4               | 1               | 2               | 8     | 0.21     | 0.44    | 0.11                | 0.18       |
| 5        | 0                    | 3               | 3               | 2               | 2               | 10    | 0.21     | 0.5     | 0.13                | 0.18       |
| 6        | 1                    | 2               | 10              | 2               | 3               | 18    | 0.14     | 0.27    | 0.04                | 0.12       |
| 7        | 0                    | 2               | 2               | 3               | 4               | 11    | 0.2      | 0.49    | 0.1                 | 0.18       |
| 8        | 1                    | 4               | 4               | 1               | 3               | 13    | 0.2      | 0.46    | 0.11                | 0.15       |
| 9        | 0                    | 0               | 8               | 2               | 2               | 12    | 0.2      | 0.37    | 0.08                | 0.18       |
| 10       | 0                    | 2               | 6               | 5               | 0               | 13    | 0.17     | 0.32    | 0.07                | 0.14       |

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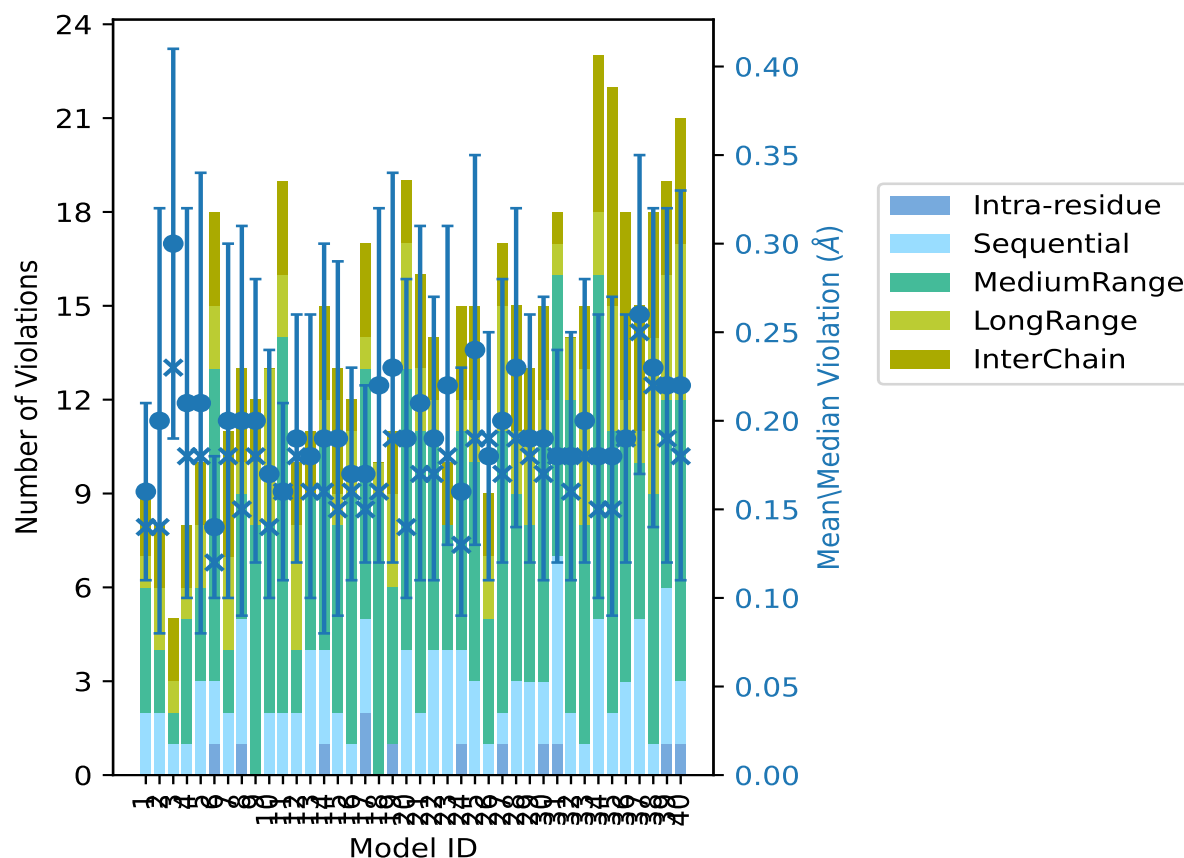
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 0                    | 2               | 12              | 2               | 3               | 19    | 0.16     | 0.3     | 0.05                | 0.16       |
| 12       | 0                    | 2               | 2               | 4               | 2               | 10    | 0.19     | 0.32    | 0.07                | 0.18       |
| 13       | 0                    | 4               | 5               | 0               | 2               | 11    | 0.18     | 0.4     | 0.08                | 0.16       |
| 14       | 1                    | 3               | 7               | 1               | 3               | 15    | 0.19     | 0.46    | 0.11                | 0.16       |
| 15       | 0                    | 2               | 6               | 1               | 4               | 13    | 0.19     | 0.49    | 0.1                 | 0.15       |
| 16       | 0                    | 1               | 8               | 2               | 1               | 12    | 0.17     | 0.36    | 0.06                | 0.16       |
| 17       | 2                    | 3               | 8               | 1               | 3               | 17    | 0.17     | 0.26    | 0.05                | 0.15       |
| 18       | 0                    | 0               | 9               | 1               | 0               | 10    | 0.22     | 0.42    | 0.1                 | 0.16       |
| 19       | 1                    | 0               | 5               | 3               | 2               | 11    | 0.23     | 0.46    | 0.11                | 0.19       |
| 20       | 0                    | 4               | 9               | 4               | 2               | 19    | 0.19     | 0.43    | 0.09                | 0.14       |
| 21       | 0                    | 2               | 9               | 2               | 3               | 16    | 0.21     | 0.4     | 0.1                 | 0.17       |
| 22       | 0                    | 4               | 7               | 1               | 2               | 14    | 0.19     | 0.32    | 0.08                | 0.17       |
| 23       | 0                    | 4               | 4               | 0               | 2               | 10    | 0.22     | 0.39    | 0.09                | 0.18       |
| 24       | 1                    | 3               | 7               | 1               | 3               | 15    | 0.16     | 0.34    | 0.07                | 0.13       |
| 25       | 0                    | 3               | 7               | 2               | 3               | 15    | 0.24     | 0.49    | 0.11                | 0.19       |
| 26       | 0                    | 1               | 4               | 2               | 2               | 9     | 0.18     | 0.29    | 0.07                | 0.19       |
| 27       | 1                    | 1               | 9               | 4               | 2               | 17    | 0.2      | 0.43    | 0.08                | 0.17       |
| 28       | 0                    | 3               | 6               | 2               | 4               | 15    | 0.23     | 0.38    | 0.09                | 0.19       |
| 29       | 0                    | 3               | 5               | 3               | 2               | 13    | 0.19     | 0.35    | 0.07                | 0.18       |
| 30       | 1                    | 2               | 8               | 1               | 3               | 15    | 0.19     | 0.41    | 0.08                | 0.17       |
| 31       | 1                    | 6               | 9               | 1               | 1               | 18    | 0.18     | 0.29    | 0.06                | 0.18       |
| 32       | 0                    | 2               | 10              | 2               | 0               | 14    | 0.18     | 0.4     | 0.07                | 0.16       |
| 33       | 0                    | 1               | 7               | 5               | 2               | 15    | 0.2      | 0.41    | 0.08                | 0.18       |
| 34       | 0                    | 5               | 11              | 2               | 5               | 23    | 0.18     | 0.34    | 0.08                | 0.15       |
| 35       | 0                    | 2               | 9               | 4               | 7               | 22    | 0.18     | 0.42    | 0.09                | 0.15       |
| 36       | 0                    | 3               | 8               | 1               | 6               | 18    | 0.19     | 0.34    | 0.07                | 0.19       |
| 37       | 0                    | 5               | 5               | 1               | 4               | 15    | 0.26     | 0.45    | 0.09                | 0.25       |
| 38       | 0                    | 1               | 8               | 5               | 4               | 18    | 0.23     | 0.43    | 0.09                | 0.22       |
| 39       | 1                    | 5               | 6               | 4               | 3               | 19    | 0.22     | 0.46    | 0.1                 | 0.19       |
| 40       | 1                    | 2               | 9               | 5               | 4               | 21    | 0.22     | 0.49    | 0.11                | 0.18       |

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

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 482(IR:171, SQ:125, MR:102, LR:35, IC:49) 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                             | 14              | 7               | 5               | 13              | 43    | 1                        | 2.5  |
| 1                             | 2               | 5               | 3               | 2               | 13    | 2                        | 5.0  |
| 2                             | 7               | 2               | 0               | 2               | 13    | 3                        | 7.5  |
| 0                             | 1               | 2               | 2               | 2               | 7     | 4                        | 10.0 |
| 0                             | 2               | 1               | 3               | 1               | 7     | 5                        | 12.5 |
| 0                             | 2               | 3               | 4               | 0               | 9     | 6                        | 15.0 |

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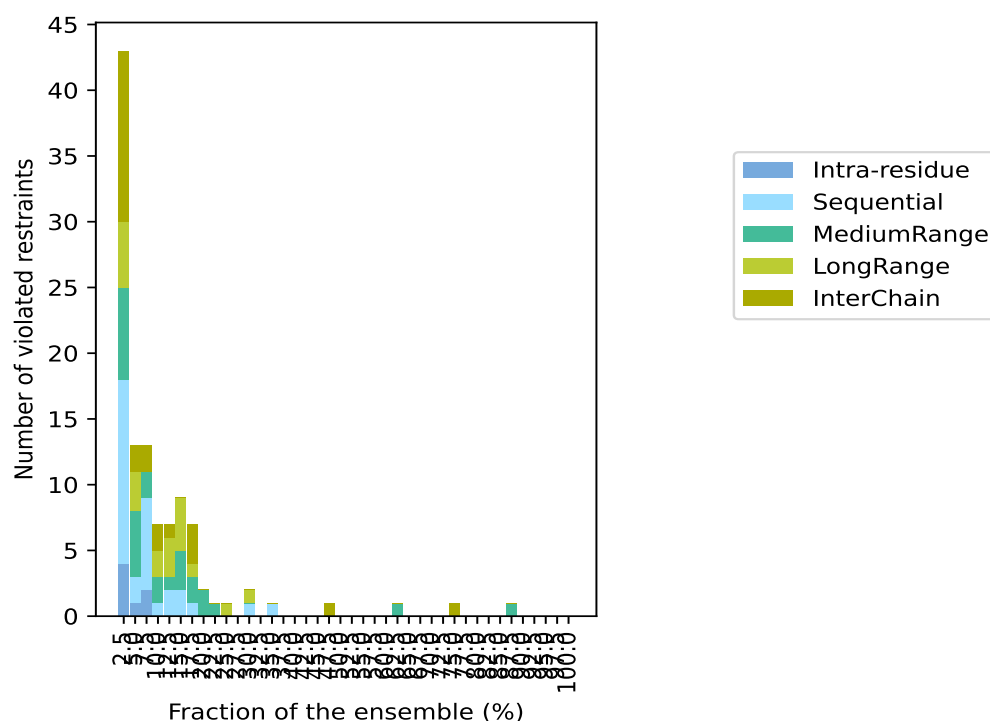
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 0                             | 1               | 2               | 1               | 3               | 7     | 7                        | 17.5  |
| 0                             | 0               | 2               | 0               | 0               | 2     | 8                        | 20.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 9                        | 22.5  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 10                       | 25.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 27.5  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 12                       | 30.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 13                       | 32.5  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 14                       | 35.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 15                       | 37.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 16                       | 40.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 42.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 18                       | 45.0  |
| 0                             | 0               | 0               | 0               | 1               | 1     | 19                       | 47.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 20                       | 50.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 21                       | 52.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 22                       | 55.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 23                       | 57.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 24                       | 60.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 25                       | 62.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 26                       | 65.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 27                       | 67.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 28                       | 70.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 29                       | 72.5  |
| 0                             | 0               | 0               | 0               | 1               | 1     | 30                       | 75.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 31                       | 77.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 32                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 33                       | 82.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 34                       | 85.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 35                       | 87.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 36                       | 90.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 37                       | 92.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 38                       | 95.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 39                       | 97.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 40                       | 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

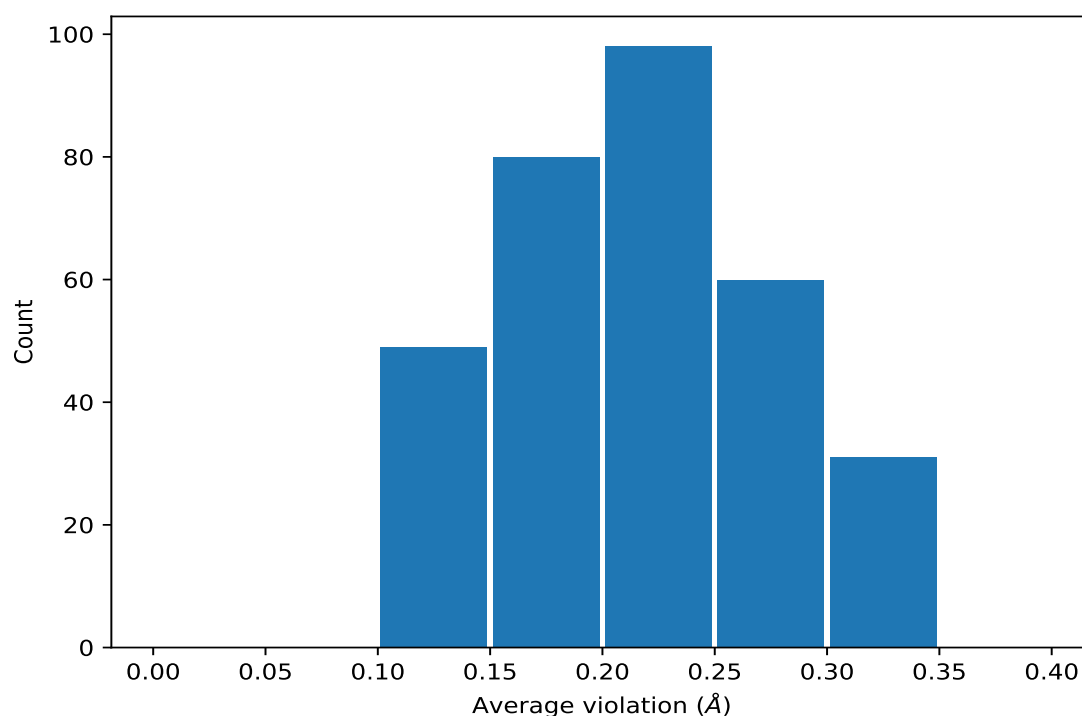
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD11 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD12 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD13 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD21 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD22 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD23 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD11 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD12 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD13 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD21 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD22 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD23 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD11 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD12 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD13 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD21 | 35                  | 0.33     | 0.1                 | 0.34       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 35                  | 0.33     | 0.1                 | 0.34       |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 30                  | 0.2      | 0.06                | 0.18       |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 30                  | 0.2      | 0.06                | 0.18       |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 30                  | 0.2      | 0.06                | 0.18       |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 25                  | 0.17     | 0.05                | 0.17       |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 25                  | 0.17     | 0.05                | 0.17       |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 25                  | 0.17     | 0.05                | 0.17       |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 19                  | 0.26     | 0.12                | 0.23       |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 19                  | 0.26     | 0.12                | 0.23       |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 19                  | 0.26     | 0.12                | 0.23       |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 19                  | 0.26     | 0.12                | 0.23       |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 19                  | 0.26     | 0.12                | 0.23       |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 19                  | 0.26     | 0.12                | 0.23       |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H    | 17                  | 0.16     | 0.07                | 0.14       |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H    | 17                  | 0.15     | 0.03                | 0.14       |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG11 | 14                  | 0.28     | 0.11                | 0.29       |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG12 | 14                  | 0.28     | 0.11                | 0.29       |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG13 | 14                  | 0.28     | 0.11                | 0.29       |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG21 | 14                  | 0.28     | 0.11                | 0.29       |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG22 | 14                  | 0.28     | 0.11                | 0.29       |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG23 | 14                  | 0.28     | 0.11                | 0.29       |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE1  | 12                  | 0.28     | 0.11                | 0.28       |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE2  | 12                  | 0.28     | 0.11                | 0.28       |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE1  | 12                  | 0.28     | 0.11                | 0.28       |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE2  | 12                  | 0.28     | 0.11                | 0.28       |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE1  | 12                  | 0.28     | 0.11                | 0.28       |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE2  | 12                  | 0.28     | 0.11                | 0.28       |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE1  | 12                  | 0.28     | 0.11                | 0.28       |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE2  | 12                  | 0.28     | 0.11                | 0.28       |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE1  | 12                  | 0.28     | 0.11                | 0.28       |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE2  | 12                  | 0.28     | 0.11                | 0.28       |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE1  | 12                  | 0.28     | 0.11                | 0.28       |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE2  | 12                  | 0.28     | 0.11                | 0.28       |
| (1,17)  | 2:48:B:VAL:HG21 | 2:49:B:CYS:H    | 12                  | 0.17     | 0.04                | 0.16       |
| (1,17)  | 2:48:B:VAL:HG22 | 2:49:B:CYS:H    | 12                  | 0.17     | 0.04                | 0.16       |
| (1,17)  | 2:48:B:VAL:HG23 | 2:49:B:CYS:H    | 12                  | 0.17     | 0.04                | 0.16       |
| (3,17)  | 1:17:A:GLU:O    | 1:20:A:CYS:H    | 11                  | 0.14     | 0.02                | 0.13       |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB2  | 10                  | 0.22     | 0.08                | 0.22       |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB3  | 10                  | 0.22     | 0.08                | 0.22       |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB2  | 10                  | 0.22     | 0.08                | 0.22       |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB3  | 10                  | 0.22     | 0.08                | 0.22       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB2  | 10                  | 0.22     | 0.08                | 0.22       |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB3  | 10                  | 0.22     | 0.08                | 0.22       |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB2  | 10                  | 0.22     | 0.08                | 0.22       |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB3  | 10                  | 0.22     | 0.08                | 0.22       |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB2  | 10                  | 0.22     | 0.08                | 0.22       |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB3  | 10                  | 0.22     | 0.08                | 0.22       |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB2  | 10                  | 0.22     | 0.08                | 0.22       |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB3  | 10                  | 0.22     | 0.08                | 0.22       |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD11 | 9                   | 0.19     | 0.06                | 0.2        |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD12 | 9                   | 0.19     | 0.06                | 0.2        |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD13 | 9                   | 0.19     | 0.06                | 0.2        |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD11 | 8                   | 0.24     | 0.08                | 0.22       |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD12 | 8                   | 0.24     | 0.08                | 0.22       |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD13 | 8                   | 0.24     | 0.08                | 0.22       |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD21 | 8                   | 0.24     | 0.08                | 0.22       |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD22 | 8                   | 0.24     | 0.08                | 0.22       |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD23 | 8                   | 0.24     | 0.08                | 0.22       |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE1  | 8                   | 0.2      | 0.07                | 0.18       |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE2  | 8                   | 0.2      | 0.07                | 0.18       |
| (3,7)   | 2:43:B:GLU:O    | 2:47:B:LEU:H    | 8                   | 0.13     | 0.03                | 0.12       |
| (1,18)  | 2:48:B:VAL:HG11 | 2:49:B:CYS:H    | 7                   | 0.24     | 0.04                | 0.27       |
| (1,18)  | 2:48:B:VAL:HG12 | 2:49:B:CYS:H    | 7                   | 0.24     | 0.04                | 0.27       |
| (1,18)  | 2:48:B:VAL:HG13 | 2:49:B:CYS:H    | 7                   | 0.24     | 0.04                | 0.27       |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG21 | 7                   | 0.21     | 0.07                | 0.18       |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG22 | 7                   | 0.21     | 0.07                | 0.18       |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG23 | 7                   | 0.21     | 0.07                | 0.18       |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD11 | 7                   | 0.2      | 0.07                | 0.17       |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD12 | 7                   | 0.2      | 0.07                | 0.17       |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD13 | 7                   | 0.2      | 0.07                | 0.17       |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD21 | 7                   | 0.2      | 0.07                | 0.17       |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD22 | 7                   | 0.2      | 0.07                | 0.17       |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD23 | 7                   | 0.2      | 0.07                | 0.17       |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD1  | 7                   | 0.18     | 0.06                | 0.15       |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD2  | 7                   | 0.18     | 0.06                | 0.15       |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD1  | 7                   | 0.18     | 0.06                | 0.15       |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD2  | 7                   | 0.18     | 0.06                | 0.15       |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD1  | 7                   | 0.18     | 0.06                | 0.15       |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD2  | 7                   | 0.18     | 0.06                | 0.15       |
| (1,6)   | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 7                   | 0.16     | 0.02                | 0.15       |
| (1,6)   | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 7                   | 0.16     | 0.02                | 0.15       |
| (1,6)   | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 7                   | 0.16     | 0.02                | 0.15       |
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE1  | 7                   | 0.15     | 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) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE2  | 7                   | 0.15     | 0.02                | 0.14       |
| (3,5)   | 2:44:B:ALA:O    | 2:48:B:VAL:H    | 7                   | 0.15     | 0.04                | 0.12       |
| (1,327) | 2:43:B:GLU:H    | 2:45:B:LEU:HB2  | 7                   | 0.14     | 0.04                | 0.14       |
| (3,3)   | 2:45:B:LEU:O    | 2:49:B:CYS:H    | 7                   | 0.13     | 0.02                | 0.13       |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG21 | 6                   | 0.24     | 0.1                 | 0.2        |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG22 | 6                   | 0.24     | 0.1                 | 0.2        |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG23 | 6                   | 0.24     | 0.1                 | 0.2        |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG21 | 6                   | 0.24     | 0.1                 | 0.2        |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG22 | 6                   | 0.24     | 0.1                 | 0.2        |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG23 | 6                   | 0.24     | 0.1                 | 0.2        |
| (1,537) | 2:49:B:CYS:HB2  | 2:50:B:GLY:H    | 6                   | 0.22     | 0.06                | 0.2        |
| (1,537) | 2:49:B:CYS:HB3  | 2:50:B:GLY:H    | 6                   | 0.22     | 0.06                | 0.2        |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE1  | 6                   | 0.2      | 0.08                | 0.18       |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE2  | 6                   | 0.2      | 0.08                | 0.18       |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE1  | 6                   | 0.2      | 0.08                | 0.18       |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE2  | 6                   | 0.2      | 0.08                | 0.18       |
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE1  | 6                   | 0.2      | 0.08                | 0.18       |
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE2  | 6                   | 0.2      | 0.08                | 0.18       |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE1  | 6                   | 0.2      | 0.07                | 0.18       |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE2  | 6                   | 0.2      | 0.07                | 0.18       |
| (3,1)   | 2:46:B:TYR:O    | 2:50:B:GLY:H    | 6                   | 0.19     | 0.07                | 0.18       |
| (1,416) | 1:12:A:SER:HB2  | 1:14:A:TYR:HD1  | 6                   | 0.17     | 0.06                | 0.17       |
| (1,416) | 1:12:A:SER:HB2  | 1:14:A:TYR:HD2  | 6                   | 0.17     | 0.06                | 0.17       |
| (1,416) | 1:12:A:SER:HB3  | 1:14:A:TYR:HD1  | 6                   | 0.17     | 0.06                | 0.17       |
| (1,416) | 1:12:A:SER:HB3  | 1:14:A:TYR:HD2  | 6                   | 0.17     | 0.06                | 0.17       |
| (1,375) | 2:45:B:LEU:HA   | 2:48:B:VAL:HB   | 6                   | 0.16     | 0.04                | 0.18       |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG11 | 6                   | 0.15     | 0.05                | 0.13       |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG12 | 6                   | 0.15     | 0.05                | 0.13       |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG13 | 6                   | 0.15     | 0.05                | 0.13       |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG21 | 6                   | 0.15     | 0.05                | 0.13       |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG22 | 6                   | 0.15     | 0.05                | 0.13       |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG23 | 6                   | 0.15     | 0.05                | 0.13       |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB2  | 6                   | 0.15     | 0.03                | 0.15       |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB3  | 6                   | 0.15     | 0.03                | 0.15       |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB2  | 6                   | 0.15     | 0.03                | 0.15       |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB3  | 6                   | 0.15     | 0.03                | 0.15       |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB2  | 6                   | 0.15     | 0.03                | 0.15       |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB3  | 6                   | 0.15     | 0.03                | 0.15       |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB2  | 6                   | 0.15     | 0.03                | 0.15       |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB3  | 6                   | 0.15     | 0.03                | 0.15       |
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB2  | 6                   | 0.15     | 0.03                | 0.15       |
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB3  | 6                   | 0.15     | 0.03                | 0.15       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB2  | 6                   | 0.15     | 0.03                | 0.15       |
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB3  | 6                   | 0.15     | 0.03                | 0.15       |
| (3,31)  | 1:1:A:GLY:O     | 1:5:A:GLN:H     | 6                   | 0.14     | 0.02                | 0.13       |
| (1,127) | 2:37:B:CYS:H    | 2:40:B:HIS:HB3  | 6                   | 0.13     | 0.03                | 0.12       |
| (3,11)  | 2:41:B:LEU:O    | 2:45:B:LEU:H    | 6                   | 0.12     | 0.01                | 0.12       |
| (1,563) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HE1  | 5                   | 0.29     | 0.05                | 0.29       |
| (1,563) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HE2  | 5                   | 0.29     | 0.05                | 0.29       |
| (1,563) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HE1  | 5                   | 0.29     | 0.05                | 0.29       |
| (1,563) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HE2  | 5                   | 0.29     | 0.05                | 0.29       |
| (1,563) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HE1  | 5                   | 0.29     | 0.05                | 0.29       |
| (1,563) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HE2  | 5                   | 0.29     | 0.05                | 0.29       |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD11 | 5                   | 0.26     | 0.12                | 0.19       |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD12 | 5                   | 0.26     | 0.12                | 0.19       |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD13 | 5                   | 0.26     | 0.12                | 0.19       |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD21 | 5                   | 0.26     | 0.12                | 0.19       |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD22 | 5                   | 0.26     | 0.12                | 0.19       |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD23 | 5                   | 0.26     | 0.12                | 0.19       |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD11 | 5                   | 0.26     | 0.12                | 0.19       |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD12 | 5                   | 0.26     | 0.12                | 0.19       |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD13 | 5                   | 0.26     | 0.12                | 0.19       |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD21 | 5                   | 0.26     | 0.12                | 0.19       |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD22 | 5                   | 0.26     | 0.12                | 0.19       |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD23 | 5                   | 0.26     | 0.12                | 0.19       |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG11 | 5                   | 0.23     | 0.13                | 0.21       |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG12 | 5                   | 0.23     | 0.13                | 0.21       |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG13 | 5                   | 0.23     | 0.13                | 0.21       |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG11 | 5                   | 0.23     | 0.13                | 0.21       |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG12 | 5                   | 0.23     | 0.13                | 0.21       |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG13 | 5                   | 0.23     | 0.13                | 0.21       |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG11 | 5                   | 0.18     | 0.06                | 0.17       |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG12 | 5                   | 0.18     | 0.06                | 0.17       |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG13 | 5                   | 0.18     | 0.06                | 0.17       |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG21 | 5                   | 0.18     | 0.06                | 0.17       |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG22 | 5                   | 0.18     | 0.06                | 0.17       |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG23 | 5                   | 0.18     | 0.06                | 0.17       |
| (1,493) | 2:39:B:SER:HB2  | 2:40:B:HIS:HD2  | 5                   | 0.17     | 0.06                | 0.15       |
| (1,493) | 2:39:B:SER:HB3  | 2:40:B:HIS:HD2  | 5                   | 0.17     | 0.06                | 0.15       |
| (1,225) | 2:45:B:LEU:HG   | 2:54:B:PHE:HE1  | 5                   | 0.17     | 0.07                | 0.14       |
| (1,225) | 2:45:B:LEU:HG   | 2:54:B:PHE:HE2  | 5                   | 0.17     | 0.07                | 0.14       |
| (1,338) | 2:42:B:VAL:HB   | 2:54:B:PHE:HE1  | 5                   | 0.14     | 0.03                | 0.14       |
| (1,338) | 2:42:B:VAL:HB   | 2:54:B:PHE:HE2  | 5                   | 0.14     | 0.03                | 0.14       |
| (1,354) | 1:4:A:GLU:HG2   | 1:8:A:THR:HG21  | 4                   | 0.3      | 0.12                | 0.34       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,354) | 1:4:A:GLU:HG2   | 1:8:A:THR:HG22  | 4                   | 0.3      | 0.12                | 0.34       |
| (1,354) | 1:4:A:GLU:HG2   | 1:8:A:THR:HG23  | 4                   | 0.3      | 0.12                | 0.34       |
| (1,354) | 1:4:A:GLU:HG3   | 1:8:A:THR:HG21  | 4                   | 0.3      | 0.12                | 0.34       |
| (1,354) | 1:4:A:GLU:HG3   | 1:8:A:THR:HG22  | 4                   | 0.3      | 0.12                | 0.34       |
| (1,354) | 1:4:A:GLU:HG3   | 1:8:A:THR:HG23  | 4                   | 0.3      | 0.12                | 0.34       |
| (1,211) | 1:19:A:TYR:HD1  | 2:45:B:LEU:HD21 | 4                   | 0.22     | 0.07                | 0.22       |
| (1,211) | 1:19:A:TYR:HD1  | 2:45:B:LEU:HD22 | 4                   | 0.22     | 0.07                | 0.22       |
| (1,211) | 1:19:A:TYR:HD1  | 2:45:B:LEU:HD23 | 4                   | 0.22     | 0.07                | 0.22       |
| (1,211) | 1:19:A:TYR:HD2  | 2:45:B:LEU:HD21 | 4                   | 0.22     | 0.07                | 0.22       |
| (1,211) | 1:19:A:TYR:HD2  | 2:45:B:LEU:HD22 | 4                   | 0.22     | 0.07                | 0.22       |
| (1,211) | 1:19:A:TYR:HD2  | 2:45:B:LEU:HD23 | 4                   | 0.22     | 0.07                | 0.22       |
| (1,25)  | 2:36:B:LEU:HD11 | 2:45:B:LEU:H    | 4                   | 0.2      | 0.06                | 0.21       |
| (1,25)  | 2:36:B:LEU:HD12 | 2:45:B:LEU:H    | 4                   | 0.2      | 0.06                | 0.21       |
| (1,25)  | 2:36:B:LEU:HD13 | 2:45:B:LEU:H    | 4                   | 0.2      | 0.06                | 0.21       |
| (1,25)  | 2:36:B:LEU:HD21 | 2:45:B:LEU:H    | 4                   | 0.2      | 0.06                | 0.21       |
| (1,25)  | 2:36:B:LEU:HD22 | 2:45:B:LEU:H    | 4                   | 0.2      | 0.06                | 0.21       |
| (1,25)  | 2:36:B:LEU:HD23 | 2:45:B:LEU:H    | 4                   | 0.2      | 0.06                | 0.21       |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD11 | 4                   | 0.2      | 0.09                | 0.2        |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD12 | 4                   | 0.2      | 0.09                | 0.2        |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD13 | 4                   | 0.2      | 0.09                | 0.2        |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD21 | 4                   | 0.2      | 0.09                | 0.2        |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD22 | 4                   | 0.2      | 0.09                | 0.2        |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD23 | 4                   | 0.2      | 0.09                | 0.2        |
| (1,178) | 2:50:B:GLY:H    | 2:51:B:GLU:H    | 4                   | 0.19     | 0.1                 | 0.16       |
| (1,209) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HD1  | 4                   | 0.17     | 0.03                | 0.18       |
| (1,209) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HD2  | 4                   | 0.17     | 0.03                | 0.18       |
| (1,209) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HD1  | 4                   | 0.17     | 0.03                | 0.18       |
| (1,209) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HD2  | 4                   | 0.17     | 0.03                | 0.18       |
| (1,209) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HD1  | 4                   | 0.17     | 0.03                | 0.18       |
| (1,209) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HD2  | 4                   | 0.17     | 0.03                | 0.18       |
| (1,5)   | 1:10:A:ILE:HD11 | 2:35:B:HIS:HE1  | 4                   | 0.17     | 0.08                | 0.12       |
| (1,5)   | 1:10:A:ILE:HD12 | 2:35:B:HIS:HE1  | 4                   | 0.17     | 0.08                | 0.12       |
| (1,5)   | 1:10:A:ILE:HD13 | 2:35:B:HIS:HE1  | 4                   | 0.17     | 0.08                | 0.12       |
| (3,15)  | 2:39:B:SER:O    | 2:43:B:GLU:H    | 4                   | 0.14     | 0.02                | 0.13       |
| (3,27)  | 1:3:A:VAL:O     | 1:7:A:CYS:H     | 4                   | 0.13     | 0.04                | 0.12       |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD11 | 3                   | 0.35     | 0.02                | 0.35       |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD12 | 3                   | 0.35     | 0.02                | 0.35       |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD13 | 3                   | 0.35     | 0.02                | 0.35       |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD21 | 3                   | 0.35     | 0.02                | 0.35       |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD22 | 3                   | 0.35     | 0.02                | 0.35       |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD23 | 3                   | 0.35     | 0.02                | 0.35       |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD11 | 3                   | 0.35     | 0.02                | 0.35       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD12 | 3                   | 0.35     | 0.02                | 0.35       |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD13 | 3                   | 0.35     | 0.02                | 0.35       |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD21 | 3                   | 0.35     | 0.02                | 0.35       |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD22 | 3                   | 0.35     | 0.02                | 0.35       |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD23 | 3                   | 0.35     | 0.02                | 0.35       |
| (1,155) | 2:54:B:PHE:H    | 2:55:B:PHE:H    | 3                   | 0.31     | 0.07                | 0.34       |
| (1,301) | 1:10:A:ILE:HD11 | 2:33:B:ASN:HB2  | 3                   | 0.27     | 0.16                | 0.16       |
| (1,301) | 1:10:A:ILE:HD11 | 2:33:B:ASN:HB3  | 3                   | 0.27     | 0.16                | 0.16       |
| (1,301) | 1:10:A:ILE:HD12 | 2:33:B:ASN:HB2  | 3                   | 0.27     | 0.16                | 0.16       |
| (1,301) | 1:10:A:ILE:HD12 | 2:33:B:ASN:HB3  | 3                   | 0.27     | 0.16                | 0.16       |
| (1,301) | 1:10:A:ILE:HD13 | 2:33:B:ASN:HB2  | 3                   | 0.27     | 0.16                | 0.16       |
| (1,301) | 1:10:A:ILE:HD13 | 2:33:B:ASN:HB3  | 3                   | 0.27     | 0.16                | 0.16       |
| (1,566) | 1:7:A:CYS:HA    | 1:8:A:THR:HG21  | 3                   | 0.23     | 0.04                | 0.21       |
| (1,566) | 1:7:A:CYS:HA    | 1:8:A:THR:HG22  | 3                   | 0.23     | 0.04                | 0.21       |
| (1,566) | 1:7:A:CYS:HA    | 1:8:A:THR:HG23  | 3                   | 0.23     | 0.04                | 0.21       |
| (1,450) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB1  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB2  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB3  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB1  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB2  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB3  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB1  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB2  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB3  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD21 | 2:44:B:ALA:HB1  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD21 | 2:44:B:ALA:HB2  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD21 | 2:44:B:ALA:HB3  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD22 | 2:44:B:ALA:HB1  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD22 | 2:44:B:ALA:HB2  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD22 | 2:44:B:ALA:HB3  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD23 | 2:44:B:ALA:HB1  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD23 | 2:44:B:ALA:HB2  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,450) | 1:16:A:LEU:HD23 | 2:44:B:ALA:HB3  | 3                   | 0.21     | 0.15                | 0.1        |
| (1,242) | 2:54:B:PHE:H    | 2:54:B:PHE:HE1  | 3                   | 0.18     | 0.08                | 0.12       |
| (1,242) | 2:54:B:PHE:H    | 2:54:B:PHE:HE2  | 3                   | 0.18     | 0.08                | 0.12       |
| (1,136) | 2:42:B:VAL:HG11 | 2:43:B:GLU:H    | 3                   | 0.17     | 0.03                | 0.16       |
| (1,136) | 2:42:B:VAL:HG12 | 2:43:B:GLU:H    | 3                   | 0.17     | 0.03                | 0.16       |
| (1,136) | 2:42:B:VAL:HG13 | 2:43:B:GLU:H    | 3                   | 0.17     | 0.03                | 0.16       |
| (1,337) | 1:16:A:LEU:HG   | 1:19:A:TYR:HE1  | 3                   | 0.17     | 0.02                | 0.18       |
| (1,337) | 1:16:A:LEU:HG   | 1:19:A:TYR:HE2  | 3                   | 0.17     | 0.02                | 0.18       |
| (1,104) | 1:20:A:CYS:HA   | 1:21:A:ASN:H    | 3                   | 0.16     | 0.02                | 0.16       |
| (1,282) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD21 | 3                   | 0.14     | 0.02                | 0.14       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,282) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD22 | 3                   | 0.14     | 0.02                | 0.14       |
| (1,282) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD23 | 3                   | 0.14     | 0.02                | 0.14       |
| (1,233) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HA   | 3                   | 0.14     | 0.03                | 0.13       |
| (1,233) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HA   | 3                   | 0.14     | 0.03                | 0.13       |
| (1,191) | 2:54:B:PHE:HA   | 2:55:B:PHE:H    | 3                   | 0.13     | 0.01                | 0.14       |
| (3,20)  | 1:16:A:LEU:O    | 1:19:A:TYR:N    | 3                   | 0.13     | 0.01                | 0.13       |
| (1,142) | 2:42:B:VAL:HB   | 2:43:B:GLU:H    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,444) | 1:16:A:LEU:HG   | 2:45:B:LEU:HD11 | 2                   | 0.26     | 0.05                | 0.26       |
| (1,444) | 1:16:A:LEU:HG   | 2:45:B:LEU:HD12 | 2                   | 0.26     | 0.05                | 0.26       |
| (1,444) | 1:16:A:LEU:HG   | 2:45:B:LEU:HD13 | 2                   | 0.26     | 0.05                | 0.26       |
| (1,444) | 1:16:A:LEU:HG   | 2:45:B:LEU:HD21 | 2                   | 0.26     | 0.05                | 0.26       |
| (1,444) | 1:16:A:LEU:HG   | 2:45:B:LEU:HD22 | 2                   | 0.26     | 0.05                | 0.26       |
| (1,444) | 1:16:A:LEU:HG   | 2:45:B:LEU:HD23 | 2                   | 0.26     | 0.05                | 0.26       |
| (1,228) | 1:2:A:ILE:HG13  | 1:19:A:TYR:HE1  | 2                   | 0.24     | 0.04                | 0.24       |
| (1,228) | 1:2:A:ILE:HG13  | 1:19:A:TYR:HE2  | 2                   | 0.24     | 0.04                | 0.24       |
| (1,43)  | 2:46:B:TYR:HE1  | 2:53:B:GLY:H    | 2                   | 0.19     | 0.01                | 0.19       |
| (1,43)  | 2:46:B:TYR:HE2  | 2:53:B:GLY:H    | 2                   | 0.19     | 0.01                | 0.19       |
| (1,253) | 2:48:B:VAL:HG21 | 2:49:B:CYS:HA   | 2                   | 0.18     | 0.03                | 0.18       |
| (1,253) | 2:48:B:VAL:HG22 | 2:49:B:CYS:HA   | 2                   | 0.18     | 0.03                | 0.18       |
| (1,253) | 2:48:B:VAL:HG23 | 2:49:B:CYS:HA   | 2                   | 0.18     | 0.03                | 0.18       |
| (1,433) | 1:15:A:GLN:HA   | 1:18:A:ASN:HD21 | 2                   | 0.17     | 0.02                | 0.17       |
| (1,433) | 1:15:A:GLN:HA   | 1:18:A:ASN:HD22 | 2                   | 0.17     | 0.02                | 0.17       |
| (1,326) | 2:43:B:GLU:H    | 2:45:B:LEU:HB3  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,483) | 2:36:B:LEU:HB2  | 2:40:B:HIS:HB2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,483) | 2:36:B:LEU:HB2  | 2:40:B:HIS:HB3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,483) | 2:36:B:LEU:HB3  | 2:40:B:HIS:HB2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,483) | 2:36:B:LEU:HB3  | 2:40:B:HIS:HB3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG11 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG12 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG13 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG21 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG22 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG23 | 2                   | 0.16     | 0.02                | 0.16       |
| (1,352) | 1:4:A:GLU:HA    | 1:8:A:THR:HG21  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,352) | 1:4:A:GLU:HA    | 1:8:A:THR:HG22  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,352) | 1:4:A:GLU:HA    | 1:8:A:THR:HG23  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,422) | 1:13:A:LEU:HB2  | 2:31:B:PHE:HD1  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,422) | 1:13:A:LEU:HB2  | 2:31:B:PHE:HD2  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,422) | 1:13:A:LEU:HB3  | 2:31:B:PHE:HD1  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,422) | 1:13:A:LEU:HB3  | 2:31:B:PHE:HD2  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,330) | 2:45:B:LEU:HB2  | 2:54:B:PHE:HE1  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,330) | 2:45:B:LEU:HB2  | 2:54:B:PHE:HE2  | 2                   | 0.16     | 0.01                | 0.16       |

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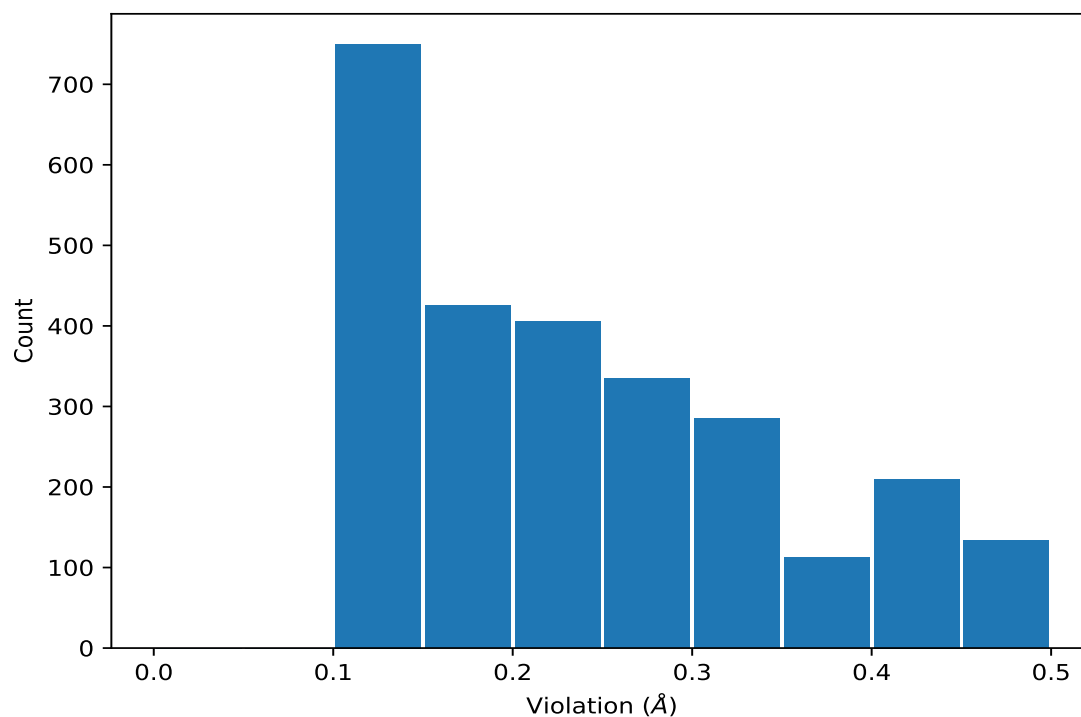
| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,84)  | 2:54:B:PHE:HB2 | 2:55:B:PHE:H    | 2                   | 0.15     | 0.04                | 0.15       |
| (3,8)   | 2:43:B:GLU:O   | 2:47:B:LEU:N    | 2                   | 0.14     | 0.04                | 0.14       |
| (3,6)   | 2:44:B:ALA:O   | 2:48:B:VAL:N    | 2                   | 0.14     | 0.02                | 0.14       |
| (1,377) | 1:13:A:LEU:HA  | 1:13:A:LEU:HD11 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,377) | 1:13:A:LEU:HA  | 1:13:A:LEU:HD12 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,377) | 1:13:A:LEU:HA  | 1:13:A:LEU:HD13 | 2                   | 0.12     | 0.02                | 0.12       |
| (3,25)  | 1:12:A:SER:O   | 1:16:A:LEU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (3,13)  | 2:40:B:HIS:O   | 2:44:B:ALA:H    | 2                   | 0.12     | 0.0                 | 0.12       |

<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) |
|---------|-----------------|-----------------|----------|---------------|
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 5        | 0.5           |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 5        | 0.5           |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE1  | 3        | 0.49          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE2  | 3        | 0.49          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE1  | 3        | 0.49          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE2  | 3        | 0.49          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE1  | 3        | 0.49          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE2  | 3        | 0.49          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE1  | 3        | 0.49          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE2  | 3        | 0.49          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE1  | 3        | 0.49          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE2  | 3        | 0.49          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE1  | 3        | 0.49          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE2  | 3        | 0.49          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 25       | 0.49          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 25       | 0.49          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 25       | 0.49          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 25       | 0.49          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 25       | 0.49          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 25       | 0.49          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 40       | 0.49          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 40       | 0.49          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 40       | 0.49          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 40       | 0.49          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 40       | 0.49          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 40       | 0.49          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 2        | 0.49          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 15       | 0.49          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 15       | 0.49          |
| (1,301) | 1:10:A:ILE:HD11 | 2:33:B:ASN:HB2  | 7        | 0.49          |
| (1,301) | 1:10:A:ILE:HD11 | 2:33:B:ASN:HB3  | 7        | 0.49          |
| (1,301) | 1:10:A:ILE:HD12 | 2:33:B:ASN:HB2  | 7        | 0.49          |
| (1,301) | 1:10:A:ILE:HD12 | 2:33:B:ASN:HB3  | 7        | 0.49          |
| (1,301) | 1:10:A:ILE:HD13 | 2:33:B:ASN:HB2  | 7        | 0.49          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,301) | 1:10:A:ILE:HD13 | 2:33:B:ASN:HB3  | 7        | 0.49          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 14       | 0.46          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 14       | 0.46          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG11 | 8        | 0.46          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG12 | 8        | 0.46          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG13 | 8        | 0.46          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG21 | 8        | 0.46          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG22 | 8        | 0.46          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG23 | 8        | 0.46          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG11 | 40       | 0.46          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG12 | 40       | 0.46          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG13 | 40       | 0.46          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG11 | 40       | 0.46          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG12 | 40       | 0.46          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG13 | 40       | 0.46          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG21 | 19       | 0.46          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG22 | 19       | 0.46          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG23 | 19       | 0.46          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG21 | 19       | 0.46          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG22 | 19       | 0.46          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG23 | 19       | 0.46          |
| (1,232) | 1:2:A:ILE:HA    | 1:19:A:TYR:HE1  | 39       | 0.46          |
| (1,232) | 1:2:A:ILE:HA    | 1:19:A:TYR:HE2  | 39       | 0.46          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD11 | 37       | 0.45          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD12 | 37       | 0.45          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD13 | 37       | 0.45          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD21 | 37       | 0.45          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD22 | 37       | 0.45          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD23 | 37       | 0.45          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD11 | 37       | 0.45          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD12 | 37       | 0.45          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD13 | 37       | 0.45          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD21 | 37       | 0.45          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD22 | 37       | 0.45          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD23 | 37       | 0.45          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG11 | 4        | 0.44          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG12 | 4        | 0.44          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG13 | 4        | 0.44          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG21 | 4        | 0.44          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG22 | 4        | 0.44          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG23 | 4        | 0.44          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB2  | 27       | 0.43          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB3  | 27       | 0.43          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB2  | 27       | 0.43          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB3  | 27       | 0.43          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB2  | 27       | 0.43          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB3  | 27       | 0.43          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB2  | 27       | 0.43          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB3  | 27       | 0.43          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB2  | 27       | 0.43          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB3  | 27       | 0.43          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB2  | 27       | 0.43          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB3  | 27       | 0.43          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 20       | 0.43          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 20       | 0.43          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 38       | 0.43          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 38       | 0.43          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE1  | 5        | 0.42          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE2  | 5        | 0.42          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE1  | 5        | 0.42          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE2  | 5        | 0.42          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE1  | 5        | 0.42          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE2  | 5        | 0.42          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE1  | 5        | 0.42          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE2  | 5        | 0.42          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE1  | 5        | 0.42          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE2  | 5        | 0.42          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE1  | 5        | 0.42          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE2  | 5        | 0.42          |
| (1,450) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB1  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB2  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB3  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB1  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB2  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB3  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB1  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB2  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB3  | 35       | 0.42          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,450) | 1:16:A:LEU:HD21 | 2:44:B:ALA:HB1  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD21 | 2:44:B:ALA:HB2  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD21 | 2:44:B:ALA:HB3  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD22 | 2:44:B:ALA:HB1  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD22 | 2:44:B:ALA:HB2  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD22 | 2:44:B:ALA:HB3  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD23 | 2:44:B:ALA:HB1  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD23 | 2:44:B:ALA:HB2  | 35       | 0.42          |
| (1,450) | 1:16:A:LEU:HD23 | 2:44:B:ALA:HB3  | 35       | 0.42          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 18       | 0.42          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 25       | 0.42          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 25       | 0.42          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 25       | 0.42          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 14       | 0.41          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 14       | 0.41          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 14       | 0.41          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 14       | 0.41          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 14       | 0.41          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 14       | 0.41          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 33       | 0.41          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 33       | 0.41          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 33       | 0.41          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 33       | 0.41          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 33       | 0.41          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 33       | 0.41          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 30       | 0.41          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 30       | 0.41          |
| (1,354) | 1:4:A:GLU:HG2   | 1:8:A:THR:HG21  | 37       | 0.41          |
| (1,354) | 1:4:A:GLU:HG2   | 1:8:A:THR:HG22  | 37       | 0.41          |
| (1,354) | 1:4:A:GLU:HG2   | 1:8:A:THR:HG23  | 37       | 0.41          |
| (1,354) | 1:4:A:GLU:HG3   | 1:8:A:THR:HG21  | 37       | 0.41          |
| (1,354) | 1:4:A:GLU:HG3   | 1:8:A:THR:HG22  | 37       | 0.41          |
| (1,354) | 1:4:A:GLU:HG3   | 1:8:A:THR:HG23  | 37       | 0.41          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 13       | 0.4           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD21 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD22 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD23 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD11 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD12 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD13 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD21 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD22 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD23 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD11 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD12 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD13 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD21 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD22 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD23 | 13       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD11 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD12 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD13 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD21 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD22 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD23 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD11 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD12 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD13 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD21 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD22 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD23 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD11 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD12 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD13 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD21 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD22 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD23 | 21       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD11 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD12 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD13 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD21 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD22 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD23 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD11 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD12 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD13 | 32       | 0.4           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD21 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD22 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD23 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD11 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD12 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD13 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD21 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD22 | 32       | 0.4           |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD23 | 32       | 0.4           |
| (1,354) | 1:4:A:GLU:HG2  | 1:8:A:THR:HG21  | 18       | 0.39          |
| (1,354) | 1:4:A:GLU:HG2  | 1:8:A:THR:HG22  | 18       | 0.39          |
| (1,354) | 1:4:A:GLU:HG2  | 1:8:A:THR:HG23  | 18       | 0.39          |
| (1,354) | 1:4:A:GLU:HG3  | 1:8:A:THR:HG21  | 18       | 0.39          |
| (1,354) | 1:4:A:GLU:HG3  | 1:8:A:THR:HG22  | 18       | 0.39          |
| (1,354) | 1:4:A:GLU:HG3  | 1:8:A:THR:HG23  | 18       | 0.39          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG11 | 21       | 0.39          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG12 | 21       | 0.39          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG13 | 21       | 0.39          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG21 | 21       | 0.39          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG22 | 21       | 0.39          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG23 | 21       | 0.39          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG11 | 23       | 0.39          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG12 | 23       | 0.39          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG13 | 23       | 0.39          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG21 | 23       | 0.39          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG22 | 23       | 0.39          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG23 | 23       | 0.39          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD11 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD12 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD13 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD21 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD22 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD23 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD11 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD12 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD13 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD21 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD22 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD23 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD11 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD12 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD13 | 8        | 0.38          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 8        | 0.38          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 19       | 0.38          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 28       | 0.38          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 28       | 0.38          |
| (1,155) | 2:54:B:PHE:H    | 2:55:B:PHE:H    | 28       | 0.38          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE1  | 21       | 0.37          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE2  | 21       | 0.37          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE1  | 21       | 0.37          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE2  | 21       | 0.37          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE1  | 21       | 0.37          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE2  | 21       | 0.37          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE1  | 21       | 0.37          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE2  | 21       | 0.37          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE1  | 21       | 0.37          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE2  | 21       | 0.37          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE1  | 21       | 0.37          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE2  | 21       | 0.37          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD11 | 37       | 0.37          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD12 | 37       | 0.37          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD13 | 37       | 0.37          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD21 | 37       | 0.37          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD22 | 37       | 0.37          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD23 | 37       | 0.37          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD11 | 9        | 0.37          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD12 | 9        | 0.37          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD13 | 9        | 0.37          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD21 | 9        | 0.37          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD22 | 9        | 0.37          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD23 | 9        | 0.37          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD11 | 9        | 0.37          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD12 | 9        | 0.37          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD13 | 9        | 0.37          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD21 | 9        | 0.37          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD22 | 9        | 0.37          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD23 | 9        | 0.37          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG21 | 40       | 0.37          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG22 | 40       | 0.37          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG23 | 40       | 0.37          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG11 | 16       | 0.36          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG12 | 16       | 0.36          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG13 | 16       | 0.36          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG21 | 16       | 0.36          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG22 | 16       | 0.36          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG23 | 16       | 0.36          |
| (1,537) | 2:49:B:CYS:HB2  | 2:50:B:GLY:H    | 38       | 0.35          |
| (1,537) | 2:49:B:CYS:HB3  | 2:50:B:GLY:H    | 38       | 0.35          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 23       | 0.35          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 23       | 0.35          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 23       | 0.35          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD11 | 25       | 0.35          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD12 | 25       | 0.35          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD13 | 25       | 0.35          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD21 | 25       | 0.35          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD22 | 25       | 0.35          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD23 | 25       | 0.35          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD11 | 25       | 0.35          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD12 | 25       | 0.35          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD13 | 25       | 0.35          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD21 | 25       | 0.35          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD22 | 25       | 0.35          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD23 | 25       | 0.35          |
| (1,178) | 2:50:B:GLY:H    | 2:51:B:GLU:H    | 29       | 0.35          |
| (1,563) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HE1  | 27       | 0.34          |
| (1,563) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HE2  | 27       | 0.34          |
| (1,563) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HE1  | 27       | 0.34          |
| (1,563) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HE2  | 27       | 0.34          |
| (1,563) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HE1  | 27       | 0.34          |
| (1,563) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HE2  | 27       | 0.34          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE1  | 39       | 0.34          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE2  | 39       | 0.34          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE1  | 39       | 0.34          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE2  | 39       | 0.34          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE1  | 39       | 0.34          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE2  | 39       | 0.34          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE1  | 39       | 0.34          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE2  | 39       | 0.34          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE1  | 39       | 0.34          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE2  | 39       | 0.34          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE1  | 39       | 0.34          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE2  | 39       | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 3        | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 24       | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 36       | 0.34          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 36       | 0.34          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 36       | 0.34          |
| (1,259) | 1:10:A:ILE:HD11 | 2:34:B:GLN:HA   | 35       | 0.34          |
| (1,259) | 1:10:A:ILE:HD12 | 2:34:B:GLN:HA   | 35       | 0.34          |
| (1,259) | 1:10:A:ILE:HD13 | 2:34:B:GLN:HA   | 35       | 0.34          |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE1  | 35       | 0.34          |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE2  | 35       | 0.34          |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE1  | 35       | 0.34          |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE2  | 35       | 0.34          |
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE1  | 35       | 0.34          |
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE2  | 35       | 0.34          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD11 | 28       | 0.34          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD12 | 28       | 0.34          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD13 | 28       | 0.34          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD21 | 28       | 0.34          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD22 | 28       | 0.34          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD23 | 28       | 0.34          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD11 | 28       | 0.34          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD12 | 28       | 0.34          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD13 | 28       | 0.34          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD21 | 28       | 0.34          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD22 | 28       | 0.34          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD23 | 28       | 0.34          |
| (1,155) | 2:54:B:PHE:H    | 2:55:B:PHE:H    | 34       | 0.34          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE1  | 38       | 0.34          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE2  | 38       | 0.34          |
| (1,563) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HE1  | 20       | 0.33          |
| (1,563) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HE2  | 20       | 0.33          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,563) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HE1  | 20       | 0.33          |
| (1,563) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HE2  | 20       | 0.33          |
| (1,563) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HE1  | 20       | 0.33          |
| (1,563) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HE2  | 20       | 0.33          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 36       | 0.33          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 36       | 0.33          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 36       | 0.33          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 33       | 0.33          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 33       | 0.33          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD11 | 39       | 0.33          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD12 | 39       | 0.33          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD13 | 39       | 0.33          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD21 | 39       | 0.33          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD22 | 39       | 0.33          |
| (1,302) | 2:43:B:GLU:HG2  | 2:47:B:LEU:HD23 | 39       | 0.33          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD11 | 39       | 0.33          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD12 | 39       | 0.33          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD13 | 39       | 0.33          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD21 | 39       | 0.33          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD22 | 39       | 0.33          |
| (1,302) | 2:43:B:GLU:HG3  | 2:47:B:LEU:HD23 | 39       | 0.33          |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H    | 39       | 0.32          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 28       | 0.32          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 28       | 0.32          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 28       | 0.32          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD11 | 22       | 0.32          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD12 | 22       | 0.32          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD13 | 22       | 0.32          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD21 | 22       | 0.32          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD22 | 22       | 0.32          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD23 | 22       | 0.32          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 22       | 0.32          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 22       | 0.32          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 22       | 0.32          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 22       | 0.32          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 22       | 0.32          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 22       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 10       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 12       | 0.32          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD12 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD13 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD21 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD22 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD23 | 12       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD11 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD12 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD13 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD21 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD22 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD23 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD11 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD12 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD13 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD21 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD22 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD23 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD11 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD12 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD13 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD21 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD22 | 39       | 0.32          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD23 | 39       | 0.32          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG11 | 22       | 0.32          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG12 | 22       | 0.32          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG13 | 22       | 0.32          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG21 | 22       | 0.32          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG22 | 22       | 0.32          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG23 | 22       | 0.32          |
| (1,211) | 1:19:A:TYR:HD1 | 2:45:B:LEU:HD21 | 34       | 0.32          |
| (1,211) | 1:19:A:TYR:HD1 | 2:45:B:LEU:HD22 | 34       | 0.32          |
| (1,211) | 1:19:A:TYR:HD1 | 2:45:B:LEU:HD23 | 34       | 0.32          |
| (1,211) | 1:19:A:TYR:HD2 | 2:45:B:LEU:HD21 | 34       | 0.32          |
| (1,211) | 1:19:A:TYR:HD2 | 2:45:B:LEU:HD22 | 34       | 0.32          |
| (1,211) | 1:19:A:TYR:HD2 | 2:45:B:LEU:HD23 | 34       | 0.32          |
| (1,444) | 1:16:A:LEU:HG  | 2:45:B:LEU:HD11 | 34       | 0.31          |
| (1,444) | 1:16:A:LEU:HG  | 2:45:B:LEU:HD12 | 34       | 0.31          |
| (1,444) | 1:16:A:LEU:HG  | 2:45:B:LEU:HD13 | 34       | 0.31          |
| (1,444) | 1:16:A:LEU:HG  | 2:45:B:LEU:HD21 | 34       | 0.31          |
| (1,444) | 1:16:A:LEU:HG  | 2:45:B:LEU:HD22 | 34       | 0.31          |
| (1,444) | 1:16:A:LEU:HG  | 2:45:B:LEU:HD23 | 34       | 0.31          |
| (1,440) | 1:16:A:LEU:HA  | 2:45:B:LEU:HD11 | 34       | 0.31          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD12 | 34       | 0.31          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD13 | 34       | 0.31          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD21 | 34       | 0.31          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD22 | 34       | 0.31          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD23 | 34       | 0.31          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 29       | 0.31          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 29       | 0.31          |
| (1,225) | 2:45:B:LEU:HG   | 2:54:B:PHE:HE1  | 38       | 0.31          |
| (1,225) | 2:45:B:LEU:HG   | 2:54:B:PHE:HE2  | 38       | 0.31          |
| (1,5)   | 1:10:A:ILE:HD11 | 2:35:B:HIS:HE1  | 37       | 0.31          |
| (1,5)   | 1:10:A:ILE:HD12 | 2:35:B:HIS:HE1  | 37       | 0.31          |
| (1,5)   | 1:10:A:ILE:HD13 | 2:35:B:HIS:HE1  | 37       | 0.31          |
| (3,1)   | 2:46:B:TYR:O    | 2:50:B:GLY:H    | 38       | 0.3           |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 14       | 0.3           |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 14       | 0.3           |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 14       | 0.3           |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE1  | 34       | 0.3           |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE2  | 34       | 0.3           |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE1  | 34       | 0.3           |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE2  | 34       | 0.3           |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE1  | 34       | 0.3           |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE2  | 34       | 0.3           |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE1  | 34       | 0.3           |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE2  | 34       | 0.3           |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE1  | 34       | 0.3           |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE2  | 34       | 0.3           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE1  | 34       | 0.3           |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE2  | 34       | 0.3           |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD11 | 11       | 0.3           |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD12 | 11       | 0.3           |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD13 | 11       | 0.3           |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD21 | 11       | 0.3           |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD22 | 11       | 0.3           |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD23 | 11       | 0.3           |
| (1,354) | 1:4:A:GLU:HG2   | 1:8:A:THR:HG21  | 25       | 0.3           |
| (1,354) | 1:4:A:GLU:HG2   | 1:8:A:THR:HG22  | 25       | 0.3           |
| (1,354) | 1:4:A:GLU:HG2   | 1:8:A:THR:HG23  | 25       | 0.3           |
| (1,354) | 1:4:A:GLU:HG3   | 1:8:A:THR:HG21  | 25       | 0.3           |
| (1,354) | 1:4:A:GLU:HG3   | 1:8:A:THR:HG22  | 25       | 0.3           |
| (1,354) | 1:4:A:GLU:HG3   | 1:8:A:THR:HG23  | 25       | 0.3           |
| (1,112) | 1:10:A:ILE:HD11 | 2:35:B:HIS:HD2  | 35       | 0.3           |
| (1,112) | 1:10:A:ILE:HD12 | 2:35:B:HIS:HD2  | 35       | 0.3           |
| (1,112) | 1:10:A:ILE:HD13 | 2:35:B:HIS:HD2  | 35       | 0.3           |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE1  | 18       | 0.3           |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE2  | 18       | 0.3           |
| (1,563) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HE1  | 8        | 0.29          |
| (1,563) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HE2  | 8        | 0.29          |
| (1,563) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HE1  | 8        | 0.29          |
| (1,563) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HE2  | 8        | 0.29          |
| (1,563) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HE1  | 8        | 0.29          |
| (1,563) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HE2  | 8        | 0.29          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 15       | 0.29          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 15       | 0.29          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 15       | 0.29          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE1  | 38       | 0.29          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE2  | 38       | 0.29          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE1  | 38       | 0.29          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE2  | 38       | 0.29          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE1  | 38       | 0.29          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE2  | 38       | 0.29          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE1  | 38       | 0.29          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE2  | 38       | 0.29          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE1  | 38       | 0.29          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE2  | 38       | 0.29          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE1  | 38       | 0.29          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE2  | 38       | 0.29          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 37       | 0.29          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 37       | 0.29          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 37       | 0.29          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 37       | 0.29          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 37       | 0.29          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 37       | 0.29          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG11 | 25       | 0.29          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG12 | 25       | 0.29          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG13 | 25       | 0.29          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG21 | 25       | 0.29          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG22 | 25       | 0.29          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG23 | 25       | 0.29          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD11 | 24       | 0.29          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD12 | 24       | 0.29          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD13 | 24       | 0.29          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD21 | 24       | 0.29          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD22 | 24       | 0.29          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD23 | 24       | 0.29          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD11 | 31       | 0.29          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD12 | 31       | 0.29          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD13 | 31       | 0.29          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD21 | 31       | 0.29          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD22 | 31       | 0.29          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD23 | 31       | 0.29          |
| (1,242) | 2:54:B:PHE:H    | 2:54:B:PHE:HE1  | 19       | 0.29          |
| (1,242) | 2:54:B:PHE:H    | 2:54:B:PHE:HE2  | 19       | 0.29          |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD1  | 26       | 0.29          |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD2  | 26       | 0.29          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD1  | 26       | 0.29          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD2  | 26       | 0.29          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD1  | 26       | 0.29          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD2  | 26       | 0.29          |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE1  | 30       | 0.29          |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE2  | 30       | 0.29          |
| (1,566) | 1:7:A:CYS:HA    | 1:8:A:THR:HG21  | 23       | 0.28          |
| (1,566) | 1:7:A:CYS:HA    | 1:8:A:THR:HG22  | 23       | 0.28          |
| (1,566) | 1:7:A:CYS:HA    | 1:8:A:THR:HG23  | 23       | 0.28          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 21       | 0.28          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 21       | 0.28          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 21       | 0.28          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 37       | 0.28          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 37       | 0.28          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 37       | 0.28          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG11 | 10       | 0.28          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG12 | 10       | 0.28          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG13 | 10       | 0.28          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG21 | 10       | 0.28          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG22 | 10       | 0.28          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG23 | 10       | 0.28          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 20       | 0.28          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 20       | 0.28          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 20       | 0.28          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 20       | 0.28          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 20       | 0.28          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 20       | 0.28          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 4        | 0.28          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 4        | 0.28          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD11 | 9        | 0.28          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD12 | 9        | 0.28          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD13 | 9        | 0.28          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 39       | 0.28          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 39       | 0.28          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 39       | 0.28          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG11 | 28       | 0.28          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG12 | 28       | 0.28          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG13 | 28       | 0.28          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG21 | 28       | 0.28          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG22 | 28       | 0.28          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG23 | 28       | 0.28          |
| (1,228) | 1:2:A:ILE:HG13  | 1:19:A:TYR:HE1  | 26       | 0.28          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,228) | 1:2:A:ILE:HG13  | 1:19:A:TYR:HE2  | 26       | 0.28          |
| (1,18)  | 2:48:B:VAL:HG11 | 2:49:B:CYS:H    | 31       | 0.28          |
| (1,18)  | 2:48:B:VAL:HG12 | 2:49:B:CYS:H    | 31       | 0.28          |
| (1,18)  | 2:48:B:VAL:HG13 | 2:49:B:CYS:H    | 31       | 0.28          |
| (3,1)   | 2:46:B:TYR:O    | 2:50:B:GLY:H    | 33       | 0.27          |
| (1,563) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HE1  | 6        | 0.27          |
| (1,563) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HE2  | 6        | 0.27          |
| (1,563) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HE1  | 6        | 0.27          |
| (1,563) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HE2  | 6        | 0.27          |
| (1,563) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HE1  | 6        | 0.27          |
| (1,563) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HE2  | 6        | 0.27          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 1        | 0.27          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 1        | 0.27          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 1        | 0.27          |
| (1,493) | 2:39:B:SER:HB2  | 2:40:B:HIS:HD2  | 31       | 0.27          |
| (1,493) | 2:39:B:SER:HB3  | 2:40:B:HIS:HD2  | 31       | 0.27          |
| (1,416) | 1:12:A:SER:HB2  | 1:14:A:TYR:HD1  | 40       | 0.27          |
| (1,416) | 1:12:A:SER:HB2  | 1:14:A:TYR:HD2  | 40       | 0.27          |
| (1,416) | 1:12:A:SER:HB3  | 1:14:A:TYR:HD1  | 40       | 0.27          |
| (1,416) | 1:12:A:SER:HB3  | 1:14:A:TYR:HD2  | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 34       | 0.27          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 40       | 0.27          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 40       | 0.27          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 40       | 0.27          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD11 | 40       | 0.27          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD12 | 40       | 0.27          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD13 | 40       | 0.27          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 33       | 0.27          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 33       | 0.27          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 33       | 0.27          |
| (1,25)  | 2:36:B:LEU:HD11 | 2:45:B:LEU:H    | 36       | 0.27          |
| (1,25)  | 2:36:B:LEU:HD12 | 2:45:B:LEU:H    | 36       | 0.27          |
| (1,25)  | 2:36:B:LEU:HD13 | 2:45:B:LEU:H    | 36       | 0.27          |
| (1,25)  | 2:36:B:LEU:HD21 | 2:45:B:LEU:H    | 36       | 0.27          |
| (1,25)  | 2:36:B:LEU:HD22 | 2:45:B:LEU:H    | 36       | 0.27          |
| (1,25)  | 2:36:B:LEU:HD23 | 2:45:B:LEU:H    | 36       | 0.27          |
| (1,18)  | 2:48:B:VAL:HG11 | 2:49:B:CYS:H    | 13       | 0.27          |
| (1,18)  | 2:48:B:VAL:HG12 | 2:49:B:CYS:H    | 13       | 0.27          |
| (1,18)  | 2:48:B:VAL:HG13 | 2:49:B:CYS:H    | 13       | 0.27          |
| (1,18)  | 2:48:B:VAL:HG11 | 2:49:B:CYS:H    | 20       | 0.27          |
| (1,18)  | 2:48:B:VAL:HG12 | 2:49:B:CYS:H    | 20       | 0.27          |
| (1,18)  | 2:48:B:VAL:HG13 | 2:49:B:CYS:H    | 20       | 0.27          |
| (1,18)  | 2:48:B:VAL:HG11 | 2:49:B:CYS:H    | 37       | 0.27          |
| (1,18)  | 2:48:B:VAL:HG12 | 2:49:B:CYS:H    | 37       | 0.27          |
| (1,18)  | 2:48:B:VAL:HG13 | 2:49:B:CYS:H    | 37       | 0.27          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE1  | 40       | 0.26          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE2  | 40       | 0.26          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE1  | 40       | 0.26          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE2  | 40       | 0.26          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE1  | 40       | 0.26          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE2  | 40       | 0.26          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE1  | 40       | 0.26          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE2  | 40       | 0.26          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE1  | 40       | 0.26          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE2  | 40       | 0.26          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE1  | 40       | 0.26          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE2  | 40       | 0.26          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB2  | 2        | 0.26          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB3  | 2        | 0.26          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB2  | 2        | 0.26          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB3  | 2        | 0.26          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB2  | 2        | 0.26          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB3  | 2        | 0.26          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB2  | 2        | 0.26          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB3  | 2        | 0.26          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB2  | 2        | 0.26          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB3  | 2        | 0.26          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB2  | 2        | 0.26          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB3  | 2        | 0.26          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD11 | 19       | 0.26          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD12 | 19       | 0.26          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD13 | 19       | 0.26          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD21 | 19       | 0.26          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD22 | 19       | 0.26          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD23 | 19       | 0.26          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 17       | 0.26          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 17       | 0.26          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 17       | 0.26          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 17       | 0.26          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 17       | 0.26          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 17       | 0.26          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD11 | 4        | 0.26          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD12 | 4        | 0.26          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD13 | 4        | 0.26          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD21 | 4        | 0.26          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD22 | 4        | 0.26          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD23 | 4        | 0.26          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD11 | 23       | 0.26          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD12 | 23       | 0.26          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD13 | 23       | 0.26          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD21 | 23       | 0.26          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD22 | 23       | 0.26          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD23 | 23       | 0.26          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 28       | 0.26          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 28       | 0.26          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 28       | 0.26          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG11 | 22       | 0.26          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG12 | 22       | 0.26          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG13 | 22       | 0.26          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG11 | 22       | 0.26          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG12 | 22       | 0.26          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG13 | 22       | 0.26          |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE1  | 40       | 0.26          |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE2  | 40       | 0.26          |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE1  | 40       | 0.26          |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE2  | 40       | 0.26          |
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE1  | 40       | 0.26          |
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE2  | 40       | 0.26          |
| (1,211) | 1:19:A:TYR:HD1  | 2:45:B:LEU:HD21 | 38       | 0.26          |
| (1,211) | 1:19:A:TYR:HD1  | 2:45:B:LEU:HD22 | 38       | 0.26          |
| (1,211) | 1:19:A:TYR:HD1  | 2:45:B:LEU:HD23 | 38       | 0.26          |
| (1,211) | 1:19:A:TYR:HD2  | 2:45:B:LEU:HD21 | 38       | 0.26          |
| (1,211) | 1:19:A:TYR:HD2  | 2:45:B:LEU:HD22 | 38       | 0.26          |
| (1,211) | 1:19:A:TYR:HD2  | 2:45:B:LEU:HD23 | 38       | 0.26          |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H    | 17       | 0.25          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 12       | 0.25          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 12       | 0.25          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 12       | 0.25          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 12       | 0.25          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 12       | 0.25          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 12       | 0.25          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 9        | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 9        | 0.25          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 31       | 0.25          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 31       | 0.25          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD11 | 37       | 0.25          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD12 | 37       | 0.25          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD13 | 37       | 0.25          |
| (1,17)  | 2:48:B:VAL:HG21 | 2:49:B:CYS:H    | 30       | 0.25          |
| (1,17)  | 2:48:B:VAL:HG22 | 2:49:B:CYS:H    | 30       | 0.25          |
| (1,17)  | 2:48:B:VAL:HG23 | 2:49:B:CYS:H    | 30       | 0.25          |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H    | 1        | 0.24          |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H    | 20       | 0.24          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 39       | 0.24          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 39       | 0.24          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 39       | 0.24          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB2  | 9        | 0.24          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB3  | 9        | 0.24          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB2  | 9        | 0.24          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB3  | 9        | 0.24          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB2  | 9        | 0.24          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB3  | 9        | 0.24          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB2  | 9        | 0.24          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB3  | 9        | 0.24          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB2  | 9        | 0.24          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB3  | 9        | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB2  | 9        | 0.24          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB3  | 9        | 0.24          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG11 | 27       | 0.24          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG12 | 27       | 0.24          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG13 | 27       | 0.24          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG21 | 27       | 0.24          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG22 | 27       | 0.24          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG23 | 27       | 0.24          |
| (1,394) | 1:2:A:ILE:HG21  | 2:45:B:LEU:HD11 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG21  | 2:45:B:LEU:HD12 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG21  | 2:45:B:LEU:HD13 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG21  | 2:45:B:LEU:HD21 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG21  | 2:45:B:LEU:HD22 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG21  | 2:45:B:LEU:HD23 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG22  | 2:45:B:LEU:HD11 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG22  | 2:45:B:LEU:HD12 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG22  | 2:45:B:LEU:HD13 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG22  | 2:45:B:LEU:HD21 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG22  | 2:45:B:LEU:HD22 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG22  | 2:45:B:LEU:HD23 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG23  | 2:45:B:LEU:HD11 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG23  | 2:45:B:LEU:HD12 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG23  | 2:45:B:LEU:HD13 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG23  | 2:45:B:LEU:HD21 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG23  | 2:45:B:LEU:HD22 | 39       | 0.24          |
| (1,394) | 1:2:A:ILE:HG23  | 2:45:B:LEU:HD23 | 39       | 0.24          |
| (1,379) | 1:13:A:LEU:HD21 | 2:31:B:PHE:HB2  | 17       | 0.24          |
| (1,379) | 1:13:A:LEU:HD21 | 2:31:B:PHE:HB3  | 17       | 0.24          |
| (1,379) | 1:13:A:LEU:HD22 | 2:31:B:PHE:HB2  | 17       | 0.24          |
| (1,379) | 1:13:A:LEU:HD22 | 2:31:B:PHE:HB3  | 17       | 0.24          |
| (1,379) | 1:13:A:LEU:HD23 | 2:31:B:PHE:HB2  | 17       | 0.24          |
| (1,379) | 1:13:A:LEU:HD23 | 2:31:B:PHE:HB3  | 17       | 0.24          |
| (1,300) | 1:10:A:ILE:HG21 | 2:33:B:ASN:HB2  | 7        | 0.24          |
| (1,300) | 1:10:A:ILE:HG21 | 2:33:B:ASN:HB3  | 7        | 0.24          |
| (1,300) | 1:10:A:ILE:HG22 | 2:33:B:ASN:HB2  | 7        | 0.24          |
| (1,300) | 1:10:A:ILE:HG22 | 2:33:B:ASN:HB3  | 7        | 0.24          |
| (1,300) | 1:10:A:ILE:HG23 | 2:33:B:ASN:HB2  | 7        | 0.24          |
| (1,300) | 1:10:A:ILE:HG23 | 2:33:B:ASN:HB3  | 7        | 0.24          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG21 | 12       | 0.24          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG22 | 12       | 0.24          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG23 | 12       | 0.24          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG21 | 12       | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG22 | 12       | 0.24          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG23 | 12       | 0.24          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE1  | 27       | 0.24          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE2  | 27       | 0.24          |
| (1,17)  | 2:48:B:VAL:HG21 | 2:49:B:CYS:H    | 17       | 0.24          |
| (1,17)  | 2:48:B:VAL:HG22 | 2:49:B:CYS:H    | 17       | 0.24          |
| (1,17)  | 2:48:B:VAL:HG23 | 2:49:B:CYS:H    | 17       | 0.24          |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H    | 38       | 0.23          |
| (3,5)   | 2:44:B:ALA:O    | 2:48:B:VAL:H    | 27       | 0.23          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 9        | 0.23          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 9        | 0.23          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 9        | 0.23          |
| (1,537) | 2:49:B:CYS:HB2  | 2:50:B:GLY:H    | 29       | 0.23          |
| (1,537) | 2:49:B:CYS:HB3  | 2:50:B:GLY:H    | 29       | 0.23          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE1  | 25       | 0.23          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE2  | 25       | 0.23          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE1  | 25       | 0.23          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE2  | 25       | 0.23          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE1  | 25       | 0.23          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE2  | 25       | 0.23          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE1  | 25       | 0.23          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE2  | 25       | 0.23          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE1  | 25       | 0.23          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE2  | 25       | 0.23          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE1  | 25       | 0.23          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE2  | 25       | 0.23          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG11 | 17       | 0.23          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG12 | 17       | 0.23          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG13 | 17       | 0.23          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG21 | 17       | 0.23          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG22 | 17       | 0.23          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG23 | 17       | 0.23          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 2        | 0.23          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 2        | 0.23          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 2        | 0.23          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 2        | 0.23          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 2        | 0.23          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 2        | 0.23          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 30       | 0.23          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 30       | 0.23          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 30       | 0.23          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 30       | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 30       | 0.23          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 30       | 0.23          |
| (1,391) | 2:37:B:CYS:H    | 2:40:B:HIS:H    | 32       | 0.23          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG11 | 3        | 0.23          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG12 | 3        | 0.23          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG13 | 3        | 0.23          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG21 | 3        | 0.23          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG22 | 3        | 0.23          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG23 | 3        | 0.23          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG21 | 38       | 0.23          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG22 | 38       | 0.23          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG23 | 38       | 0.23          |
| (1,267) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG11 | 24       | 0.23          |
| (1,267) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG12 | 24       | 0.23          |
| (1,267) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG13 | 24       | 0.23          |
| (1,25)  | 2:36:B:LEU:HD11 | 2:45:B:LEU:H    | 12       | 0.23          |
| (1,25)  | 2:36:B:LEU:HD12 | 2:45:B:LEU:H    | 12       | 0.23          |
| (1,25)  | 2:36:B:LEU:HD13 | 2:45:B:LEU:H    | 12       | 0.23          |
| (1,25)  | 2:36:B:LEU:HD21 | 2:45:B:LEU:H    | 12       | 0.23          |
| (1,25)  | 2:36:B:LEU:HD22 | 2:45:B:LEU:H    | 12       | 0.23          |
| (1,25)  | 2:36:B:LEU:HD23 | 2:45:B:LEU:H    | 12       | 0.23          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H    | 11       | 0.22          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 30       | 0.22          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 30       | 0.22          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 30       | 0.22          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 33       | 0.22          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 33       | 0.22          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 33       | 0.22          |
| (1,537) | 2:49:B:CYS:HB2  | 2:50:B:GLY:H    | 22       | 0.22          |
| (1,537) | 2:49:B:CYS:HB3  | 2:50:B:GLY:H    | 22       | 0.22          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB2  | 7        | 0.22          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB3  | 7        | 0.22          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB2  | 7        | 0.22          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB3  | 7        | 0.22          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB2  | 7        | 0.22          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB3  | 7        | 0.22          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB2  | 7        | 0.22          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB3  | 7        | 0.22          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB2  | 7        | 0.22          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB3  | 7        | 0.22          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB2  | 7        | 0.22          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB3  | 7        | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB2  | 26       | 0.22          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB3  | 26       | 0.22          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB2  | 26       | 0.22          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB3  | 26       | 0.22          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB2  | 26       | 0.22          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB3  | 26       | 0.22          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB2  | 26       | 0.22          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB3  | 26       | 0.22          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB2  | 26       | 0.22          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB3  | 26       | 0.22          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB2  | 26       | 0.22          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB3  | 26       | 0.22          |
| (1,478) | 2:34:B:GLN:HG2  | 2:36:B:LEU:HD11 | 31       | 0.22          |
| (1,478) | 2:34:B:GLN:HG2  | 2:36:B:LEU:HD12 | 31       | 0.22          |
| (1,478) | 2:34:B:GLN:HG2  | 2:36:B:LEU:HD13 | 31       | 0.22          |
| (1,478) | 2:34:B:GLN:HG2  | 2:36:B:LEU:HD21 | 31       | 0.22          |
| (1,478) | 2:34:B:GLN:HG2  | 2:36:B:LEU:HD22 | 31       | 0.22          |
| (1,478) | 2:34:B:GLN:HG2  | 2:36:B:LEU:HD23 | 31       | 0.22          |
| (1,478) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD11 | 31       | 0.22          |
| (1,478) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD12 | 31       | 0.22          |
| (1,478) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD13 | 31       | 0.22          |
| (1,478) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD21 | 31       | 0.22          |
| (1,478) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD22 | 31       | 0.22          |
| (1,478) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD23 | 31       | 0.22          |
| (1,458) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG11 | 38       | 0.22          |
| (1,458) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG12 | 38       | 0.22          |
| (1,458) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG13 | 38       | 0.22          |
| (1,458) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG21 | 38       | 0.22          |
| (1,458) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG22 | 38       | 0.22          |
| (1,458) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG23 | 38       | 0.22          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 15       | 0.22          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 15       | 0.22          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 15       | 0.22          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 15       | 0.22          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 15       | 0.22          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 15       | 0.22          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 21       | 0.22          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 21       | 0.22          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 21       | 0.22          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 21       | 0.22          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 21       | 0.22          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 21       | 0.22          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,155) | 2:54:B:PHE:H    | 2:55:B:PHE:H   | 36       | 0.22          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE1 | 21       | 0.22          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE2 | 21       | 0.22          |
| (1,18)  | 2:48:B:VAL:HG11 | 2:49:B:CYS:H   | 26       | 0.22          |
| (1,18)  | 2:48:B:VAL:HG12 | 2:49:B:CYS:H   | 26       | 0.22          |
| (1,18)  | 2:48:B:VAL:HG13 | 2:49:B:CYS:H   | 26       | 0.22          |
| (1,18)  | 2:48:B:VAL:HG11 | 2:49:B:CYS:H   | 27       | 0.22          |
| (1,18)  | 2:48:B:VAL:HG12 | 2:49:B:CYS:H   | 27       | 0.22          |
| (1,18)  | 2:48:B:VAL:HG13 | 2:49:B:CYS:H   | 27       | 0.22          |
| (1,17)  | 2:48:B:VAL:HG21 | 2:49:B:CYS:H   | 32       | 0.22          |
| (1,17)  | 2:48:B:VAL:HG22 | 2:49:B:CYS:H   | 32       | 0.22          |
| (1,17)  | 2:48:B:VAL:HG23 | 2:49:B:CYS:H   | 32       | 0.22          |
| (1,566) | 1:7:A:CYS:HA    | 1:8:A:THR:HG21 | 37       | 0.21          |
| (1,566) | 1:7:A:CYS:HA    | 1:8:A:THR:HG22 | 37       | 0.21          |
| (1,566) | 1:7:A:CYS:HA    | 1:8:A:THR:HG23 | 37       | 0.21          |
| (1,563) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HE1 | 3        | 0.21          |
| (1,563) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HE2 | 3        | 0.21          |
| (1,563) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HE1 | 3        | 0.21          |
| (1,563) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HE2 | 3        | 0.21          |
| (1,563) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HE1 | 3        | 0.21          |
| (1,563) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HE2 | 3        | 0.21          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1 | 19       | 0.21          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1 | 19       | 0.21          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1 | 19       | 0.21          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE1 | 29       | 0.21          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE2 | 29       | 0.21          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE1 | 29       | 0.21          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE2 | 29       | 0.21          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE1 | 29       | 0.21          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE2 | 29       | 0.21          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE1 | 29       | 0.21          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE2 | 29       | 0.21          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE1 | 29       | 0.21          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE2 | 29       | 0.21          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE1 | 29       | 0.21          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE2 | 29       | 0.21          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB2 | 40       | 0.21          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB3 | 40       | 0.21          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB2 | 40       | 0.21          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB3 | 40       | 0.21          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB2 | 40       | 0.21          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB3 | 40       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB2  | 40       | 0.21          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB3  | 40       | 0.21          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB2  | 40       | 0.21          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB3  | 40       | 0.21          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB2  | 40       | 0.21          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB3  | 40       | 0.21          |
| (1,444) | 1:16:A:LEU:HG   | 2:45:B:LEU:HD11 | 3        | 0.21          |
| (1,444) | 1:16:A:LEU:HG   | 2:45:B:LEU:HD12 | 3        | 0.21          |
| (1,444) | 1:16:A:LEU:HG   | 2:45:B:LEU:HD13 | 3        | 0.21          |
| (1,444) | 1:16:A:LEU:HG   | 2:45:B:LEU:HD21 | 3        | 0.21          |
| (1,444) | 1:16:A:LEU:HG   | 2:45:B:LEU:HD22 | 3        | 0.21          |
| (1,444) | 1:16:A:LEU:HG   | 2:45:B:LEU:HD23 | 3        | 0.21          |
| (1,422) | 1:13:A:LEU:HB2  | 2:31:B:PHE:HD1  | 11       | 0.21          |
| (1,422) | 1:13:A:LEU:HB2  | 2:31:B:PHE:HD2  | 11       | 0.21          |
| (1,422) | 1:13:A:LEU:HB3  | 2:31:B:PHE:HD1  | 11       | 0.21          |
| (1,422) | 1:13:A:LEU:HB3  | 2:31:B:PHE:HD2  | 11       | 0.21          |
| (1,416) | 1:12:A:SER:HB2  | 1:14:A:TYR:HD1  | 28       | 0.21          |
| (1,416) | 1:12:A:SER:HB2  | 1:14:A:TYR:HD2  | 28       | 0.21          |
| (1,416) | 1:12:A:SER:HB3  | 1:14:A:TYR:HD1  | 28       | 0.21          |
| (1,416) | 1:12:A:SER:HB3  | 1:14:A:TYR:HD2  | 28       | 0.21          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 27       | 0.21          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 27       | 0.21          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD11 | 16       | 0.21          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD12 | 16       | 0.21          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD13 | 16       | 0.21          |
| (1,375) | 2:45:B:LEU:HA   | 2:48:B:VAL:HB   | 20       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 12       | 0.21          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 12       | 0.21          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 12       | 0.21          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 15       | 0.21          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 15       | 0.21          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 15       | 0.21          |
| (1,314) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB1  | 36       | 0.21          |
| (1,314) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB2  | 36       | 0.21          |
| (1,314) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB3  | 36       | 0.21          |
| (1,314) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB1  | 36       | 0.21          |
| (1,314) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB2  | 36       | 0.21          |
| (1,314) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB3  | 36       | 0.21          |
| (1,314) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB1  | 36       | 0.21          |
| (1,314) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB2  | 36       | 0.21          |
| (1,314) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB3  | 36       | 0.21          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG11 | 7        | 0.21          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG12 | 7        | 0.21          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG13 | 7        | 0.21          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG11 | 7        | 0.21          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG12 | 7        | 0.21          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG13 | 7        | 0.21          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG21 | 20       | 0.21          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG22 | 20       | 0.21          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG23 | 20       | 0.21          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG21 | 20       | 0.21          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG22 | 20       | 0.21          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG23 | 20       | 0.21          |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD1  | 36       | 0.21          |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD2  | 36       | 0.21          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD1  | 36       | 0.21          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD2  | 36       | 0.21          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD1  | 36       | 0.21          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD2  | 36       | 0.21          |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD1  | 37       | 0.21          |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD2  | 37       | 0.21          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD1  | 37       | 0.21          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD2  | 37       | 0.21          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD1  | 37       | 0.21          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD2  | 37       | 0.21          |
| (1,136) | 2:42:B:VAL:HG11 | 2:43:B:GLU:H    | 39       | 0.21          |
| (1,136) | 2:42:B:VAL:HG12 | 2:43:B:GLU:H    | 39       | 0.21          |
| (1,136) | 2:42:B:VAL:HG13 | 2:43:B:GLU:H    | 39       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,27)  | 1:3:A:VAL:O     | 1:7:A:CYS:H     | 21       | 0.2           |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H    | 10       | 0.2           |
| (1,566) | 1:7:A:CYS:HA    | 1:8:A:THR:HG21  | 36       | 0.2           |
| (1,566) | 1:7:A:CYS:HA    | 1:8:A:THR:HG22  | 36       | 0.2           |
| (1,566) | 1:7:A:CYS:HA    | 1:8:A:THR:HG23  | 36       | 0.2           |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 29       | 0.2           |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 29       | 0.2           |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 29       | 0.2           |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB2  | 10       | 0.2           |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB3  | 10       | 0.2           |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB2  | 10       | 0.2           |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB3  | 10       | 0.2           |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB2  | 10       | 0.2           |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB3  | 10       | 0.2           |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB2  | 10       | 0.2           |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB3  | 10       | 0.2           |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB2  | 10       | 0.2           |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB3  | 10       | 0.2           |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB2  | 10       | 0.2           |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB3  | 10       | 0.2           |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 31       | 0.2           |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 31       | 0.2           |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 31       | 0.2           |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 31       | 0.2           |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 31       | 0.2           |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 31       | 0.2           |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 11       | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 11       | 0.2           |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 11       | 0.2           |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB2  | 5        | 0.2           |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB3  | 5        | 0.2           |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB2  | 5        | 0.2           |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB3  | 5        | 0.2           |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB2  | 5        | 0.2           |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB3  | 5        | 0.2           |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB2  | 5        | 0.2           |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB3  | 5        | 0.2           |
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB2  | 5        | 0.2           |
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB3  | 5        | 0.2           |
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB2  | 5        | 0.2           |
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB3  | 5        | 0.2           |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD11 | 31       | 0.2           |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD12 | 31       | 0.2           |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD13 | 31       | 0.2           |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 4        | 0.2           |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 4        | 0.2           |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 4        | 0.2           |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 10       | 0.2           |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 10       | 0.2           |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 10       | 0.2           |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 36       | 0.2           |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 36       | 0.2           |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 36       | 0.2           |
| (1,327) | 2:43:B:GLU:H    | 2:45:B:LEU:HB2  | 40       | 0.2           |
| (1,326) | 2:43:B:GLU:H    | 2:45:B:LEU:HB3  | 32       | 0.2           |
| (1,253) | 2:48:B:VAL:HG21 | 2:49:B:CYS:HA   | 5        | 0.2           |
| (1,253) | 2:48:B:VAL:HG22 | 2:49:B:CYS:HA   | 5        | 0.2           |
| (1,253) | 2:48:B:VAL:HG23 | 2:49:B:CYS:HA   | 5        | 0.2           |
| (1,228) | 1:2:A:ILE:HG13  | 1:19:A:TYR:HE1  | 5        | 0.2           |
| (1,228) | 1:2:A:ILE:HG13  | 1:19:A:TYR:HE2  | 5        | 0.2           |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE1  | 20       | 0.2           |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE2  | 20       | 0.2           |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE1  | 20       | 0.2           |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE2  | 20       | 0.2           |
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE1  | 20       | 0.2           |
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE2  | 20       | 0.2           |
| (1,209) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HD1  | 29       | 0.2           |
| (1,209) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HD2  | 29       | 0.2           |
| (1,209) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HD1  | 29       | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,209) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HD2  | 29       | 0.2           |
| (1,209) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HD1  | 29       | 0.2           |
| (1,209) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HD2  | 29       | 0.2           |
| (1,209) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HD1  | 37       | 0.2           |
| (1,209) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HD2  | 37       | 0.2           |
| (1,209) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HD1  | 37       | 0.2           |
| (1,209) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HD2  | 37       | 0.2           |
| (1,209) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HD1  | 37       | 0.2           |
| (1,209) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HD2  | 37       | 0.2           |
| (1,178) | 2:50:B:GLY:H    | 2:51:B:GLU:H    | 37       | 0.2           |
| (1,43)  | 2:46:B:TYR:HE1  | 2:53:B:GLY:H    | 38       | 0.2           |
| (1,43)  | 2:46:B:TYR:HE2  | 2:53:B:GLY:H    | 38       | 0.2           |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H    | 11       | 0.19          |
| (3,7)   | 2:43:B:GLU:O    | 2:47:B:LEU:H    | 34       | 0.19          |
| (3,5)   | 2:44:B:ALA:O    | 2:48:B:VAL:H    | 28       | 0.19          |
| (3,1)   | 2:46:B:TYR:O    | 2:50:B:GLY:H    | 22       | 0.19          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 11       | 0.19          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 11       | 0.19          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 11       | 0.19          |
| (1,537) | 2:49:B:CYS:HB2  | 2:50:B:GLY:H    | 33       | 0.19          |
| (1,537) | 2:49:B:CYS:HB3  | 2:50:B:GLY:H    | 33       | 0.19          |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG11 | 7        | 0.19          |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG12 | 7        | 0.19          |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG13 | 7        | 0.19          |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG21 | 7        | 0.19          |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG22 | 7        | 0.19          |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG23 | 7        | 0.19          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD11 | 25       | 0.19          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD12 | 25       | 0.19          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD13 | 25       | 0.19          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD21 | 25       | 0.19          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD22 | 25       | 0.19          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD23 | 25       | 0.19          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD11 | 31       | 0.19          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD12 | 31       | 0.19          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD13 | 31       | 0.19          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD21 | 31       | 0.19          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD22 | 31       | 0.19          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD23 | 31       | 0.19          |
| (1,493) | 2:39:B:SER:HB2  | 2:40:B:HIS:HD2  | 14       | 0.19          |
| (1,493) | 2:39:B:SER:HB3  | 2:40:B:HIS:HD2  | 14       | 0.19          |
| (1,483) | 2:36:B:LEU:HB2  | 2:40:B:HIS:HB2  | 8        | 0.19          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,483) | 2:36:B:LEU:HB2 | 2:40:B:HIS:HB3  | 8        | 0.19          |
| (1,483) | 2:36:B:LEU:HB3 | 2:40:B:HIS:HB2  | 8        | 0.19          |
| (1,483) | 2:36:B:LEU:HB3 | 2:40:B:HIS:HB3  | 8        | 0.19          |
| (1,433) | 1:15:A:GLN:HA  | 1:18:A:ASN:HD21 | 21       | 0.19          |
| (1,433) | 1:15:A:GLN:HA  | 1:18:A:ASN:HD22 | 21       | 0.19          |
| (1,416) | 1:12:A:SER:HB2 | 1:14:A:TYR:HD1  | 9        | 0.19          |
| (1,416) | 1:12:A:SER:HB2 | 1:14:A:TYR:HD2  | 9        | 0.19          |
| (1,416) | 1:12:A:SER:HB3 | 1:14:A:TYR:HD1  | 9        | 0.19          |
| (1,416) | 1:12:A:SER:HB3 | 1:14:A:TYR:HD2  | 9        | 0.19          |
| (1,375) | 2:45:B:LEU:HA  | 2:48:B:VAL:HB   | 26       | 0.19          |
| (1,375) | 2:45:B:LEU:HA  | 2:48:B:VAL:HB   | 31       | 0.19          |
| (1,353) | 2:45:B:LEU:HA  | 2:48:B:VAL:HG21 | 19       | 0.19          |
| (1,353) | 2:45:B:LEU:HA  | 2:48:B:VAL:HG22 | 19       | 0.19          |
| (1,353) | 2:45:B:LEU:HA  | 2:48:B:VAL:HG23 | 19       | 0.19          |
| (1,353) | 2:45:B:LEU:HA  | 2:48:B:VAL:HG21 | 25       | 0.19          |
| (1,353) | 2:45:B:LEU:HA  | 2:48:B:VAL:HG22 | 25       | 0.19          |
| (1,353) | 2:45:B:LEU:HA  | 2:48:B:VAL:HG23 | 25       | 0.19          |
| (1,338) | 2:42:B:VAL:HB  | 2:54:B:PHE:HE1  | 11       | 0.19          |
| (1,338) | 2:42:B:VAL:HB  | 2:54:B:PHE:HE2  | 11       | 0.19          |
| (1,337) | 1:16:A:LEU:HG  | 1:19:A:TYR:HE1  | 16       | 0.19          |
| (1,337) | 1:16:A:LEU:HG  | 1:19:A:TYR:HE2  | 16       | 0.19          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG11 | 6        | 0.19          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG12 | 6        | 0.19          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG13 | 6        | 0.19          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG21 | 6        | 0.19          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG22 | 6        | 0.19          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG23 | 6        | 0.19          |
| (1,276) | 1:17:A:GLU:HA  | 2:48:B:VAL:HG21 | 36       | 0.19          |
| (1,276) | 1:17:A:GLU:HA  | 2:48:B:VAL:HG22 | 36       | 0.19          |
| (1,276) | 1:17:A:GLU:HA  | 2:48:B:VAL:HG23 | 36       | 0.19          |
| (1,246) | 2:31:B:PHE:HE1 | 2:48:B:VAL:HG21 | 33       | 0.19          |
| (1,246) | 2:31:B:PHE:HE1 | 2:48:B:VAL:HG22 | 33       | 0.19          |
| (1,246) | 2:31:B:PHE:HE1 | 2:48:B:VAL:HG23 | 33       | 0.19          |
| (1,246) | 2:31:B:PHE:HE2 | 2:48:B:VAL:HG21 | 33       | 0.19          |
| (1,246) | 2:31:B:PHE:HE2 | 2:48:B:VAL:HG22 | 33       | 0.19          |
| (1,246) | 2:31:B:PHE:HE2 | 2:48:B:VAL:HG23 | 33       | 0.19          |
| (1,229) | 1:2:A:ILE:HG12 | 1:19:A:TYR:HE1  | 27       | 0.19          |
| (1,229) | 1:2:A:ILE:HG12 | 1:19:A:TYR:HE2  | 27       | 0.19          |
| (1,211) | 1:19:A:TYR:HD1 | 2:45:B:LEU:HD21 | 28       | 0.19          |
| (1,211) | 1:19:A:TYR:HD1 | 2:45:B:LEU:HD22 | 28       | 0.19          |
| (1,211) | 1:19:A:TYR:HD1 | 2:45:B:LEU:HD23 | 28       | 0.19          |
| (1,211) | 1:19:A:TYR:HD2 | 2:45:B:LEU:HD21 | 28       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,211) | 1:19:A:TYR:HD2  | 2:45:B:LEU:HD22 | 28       | 0.19          |
| (1,211) | 1:19:A:TYR:HD2  | 2:45:B:LEU:HD23 | 28       | 0.19          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD11 | 6        | 0.19          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD12 | 6        | 0.19          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD13 | 6        | 0.19          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD21 | 6        | 0.19          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD22 | 6        | 0.19          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD23 | 6        | 0.19          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD11 | 6        | 0.19          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD12 | 6        | 0.19          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD13 | 6        | 0.19          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD21 | 6        | 0.19          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD22 | 6        | 0.19          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD23 | 6        | 0.19          |
| (1,104) | 1:20:A:CYS:HA   | 1:21:A:ASN:H    | 32       | 0.19          |
| (1,84)  | 2:54:B:PHE:HB2  | 2:55:B:PHE:H    | 25       | 0.19          |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE1  | 35       | 0.19          |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE2  | 35       | 0.19          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE1  | 25       | 0.19          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE2  | 25       | 0.19          |
| (1,25)  | 2:36:B:LEU:HD11 | 2:45:B:LEU:H    | 28       | 0.19          |
| (1,25)  | 2:36:B:LEU:HD12 | 2:45:B:LEU:H    | 28       | 0.19          |
| (1,25)  | 2:36:B:LEU:HD13 | 2:45:B:LEU:H    | 28       | 0.19          |
| (1,25)  | 2:36:B:LEU:HD21 | 2:45:B:LEU:H    | 28       | 0.19          |
| (1,25)  | 2:36:B:LEU:HD22 | 2:45:B:LEU:H    | 28       | 0.19          |
| (1,25)  | 2:36:B:LEU:HD23 | 2:45:B:LEU:H    | 28       | 0.19          |
| (1,17)  | 2:48:B:VAL:HG21 | 2:49:B:CYS:H    | 39       | 0.19          |
| (1,17)  | 2:48:B:VAL:HG22 | 2:49:B:CYS:H    | 39       | 0.19          |
| (1,17)  | 2:48:B:VAL:HG23 | 2:49:B:CYS:H    | 39       | 0.19          |
| (1,6)   | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 36       | 0.19          |
| (1,6)   | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 36       | 0.19          |
| (1,6)   | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 36       | 0.19          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H    | 6        | 0.18          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H    | 16       | 0.18          |
| (3,17)  | 1:17:A:GLU:O    | 1:20:A:CYS:H    | 30       | 0.18          |
| (3,8)   | 2:43:B:GLU:O    | 2:47:B:LEU:N    | 34       | 0.18          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 7        | 0.18          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 7        | 0.18          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 7        | 0.18          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 16       | 0.18          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 16       | 0.18          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 16       | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 17       | 0.18          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 17       | 0.18          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 17       | 0.18          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 34       | 0.18          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 34       | 0.18          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 34       | 0.18          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 40       | 0.18          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 40       | 0.18          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 40       | 0.18          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE1  | 33       | 0.18          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE2  | 33       | 0.18          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE1  | 33       | 0.18          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE2  | 33       | 0.18          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE1  | 33       | 0.18          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE2  | 33       | 0.18          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE1  | 33       | 0.18          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE2  | 33       | 0.18          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE1  | 33       | 0.18          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE2  | 33       | 0.18          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE1  | 33       | 0.18          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE2  | 33       | 0.18          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD11 | 18       | 0.18          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD12 | 18       | 0.18          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD13 | 18       | 0.18          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD21 | 18       | 0.18          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD22 | 18       | 0.18          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD23 | 18       | 0.18          |
| (1,475) | 2:34:B:GLN:H    | 2:34:B:GLN:HG2  | 31       | 0.18          |
| (1,475) | 2:34:B:GLN:H    | 2:34:B:GLN:HG3  | 31       | 0.18          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG11 | 38       | 0.18          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG12 | 38       | 0.18          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG13 | 38       | 0.18          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG21 | 38       | 0.18          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG22 | 38       | 0.18          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG23 | 38       | 0.18          |
| (1,420) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD11 | 34       | 0.18          |
| (1,420) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD12 | 34       | 0.18          |
| (1,420) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD13 | 34       | 0.18          |
| (1,420) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD21 | 34       | 0.18          |
| (1,420) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD22 | 34       | 0.18          |
| (1,420) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD23 | 34       | 0.18          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 17       | 0.18          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD12 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD13 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD21 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD22 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB1 | 2:47:B:LEU:HD23 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD11 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD12 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD13 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD21 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD22 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB2 | 2:47:B:LEU:HD23 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD11 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD12 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD13 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD21 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD22 | 17       | 0.18          |
| (1,387) | 2:44:B:ALA:HB3 | 2:47:B:LEU:HD23 | 17       | 0.18          |
| (1,353) | 2:45:B:LEU:HA  | 2:48:B:VAL:HG21 | 1        | 0.18          |
| (1,353) | 2:45:B:LEU:HA  | 2:48:B:VAL:HG22 | 1        | 0.18          |
| (1,353) | 2:45:B:LEU:HA  | 2:48:B:VAL:HG23 | 1        | 0.18          |
| (1,353) | 2:45:B:LEU:HA  | 2:48:B:VAL:HG21 | 23       | 0.18          |
| (1,353) | 2:45:B:LEU:HA  | 2:48:B:VAL:HG22 | 23       | 0.18          |
| (1,353) | 2:45:B:LEU:HA  | 2:48:B:VAL:HG23 | 23       | 0.18          |
| (1,352) | 1:4:A:GLU:HA   | 1:8:A:THR:HG21  | 11       | 0.18          |
| (1,352) | 1:4:A:GLU:HA   | 1:8:A:THR:HG22  | 11       | 0.18          |
| (1,352) | 1:4:A:GLU:HA   | 1:8:A:THR:HG23  | 11       | 0.18          |
| (1,337) | 1:16:A:LEU:HG  | 1:19:A:TYR:HE1  | 13       | 0.18          |
| (1,337) | 1:16:A:LEU:HG  | 1:19:A:TYR:HE2  | 13       | 0.18          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG11 | 11       | 0.18          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG12 | 11       | 0.18          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG13 | 11       | 0.18          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG21 | 11       | 0.18          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG22 | 11       | 0.18          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG23 | 11       | 0.18          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG11 | 13       | 0.18          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG12 | 13       | 0.18          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG13 | 13       | 0.18          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG21 | 13       | 0.18          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG22 | 13       | 0.18          |
| (1,328) | 2:31:B:PHE:HZ  | 2:32:B:VAL:HG23 | 13       | 0.18          |
| (1,327) | 2:43:B:GLU:H   | 2:45:B:LEU:HB2  | 33       | 0.18          |
| (1,276) | 1:17:A:GLU:HA  | 2:48:B:VAL:HG21 | 7        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG22 | 7        | 0.18          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG23 | 7        | 0.18          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG21 | 8        | 0.18          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG22 | 8        | 0.18          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG23 | 8        | 0.18          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG21 | 22       | 0.18          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG22 | 22       | 0.18          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG23 | 22       | 0.18          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG21 | 28       | 0.18          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG22 | 28       | 0.18          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG23 | 28       | 0.18          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG21 | 28       | 0.18          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG22 | 28       | 0.18          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG23 | 28       | 0.18          |
| (1,233) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HA   | 37       | 0.18          |
| (1,233) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HA   | 37       | 0.18          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD11 | 17       | 0.18          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD12 | 17       | 0.18          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD13 | 17       | 0.18          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD21 | 17       | 0.18          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD22 | 17       | 0.18          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD23 | 17       | 0.18          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD11 | 17       | 0.18          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD12 | 17       | 0.18          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD13 | 17       | 0.18          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD21 | 17       | 0.18          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD22 | 17       | 0.18          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD23 | 17       | 0.18          |
| (1,127) | 2:37:B:CYS:H    | 2:40:B:HIS:HB3  | 28       | 0.18          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE1  | 29       | 0.18          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE2  | 29       | 0.18          |
| (1,43)  | 2:46:B:TYR:HE1  | 2:53:B:GLY:H    | 40       | 0.18          |
| (1,43)  | 2:46:B:TYR:HE2  | 2:53:B:GLY:H    | 40       | 0.18          |
| (1,6)   | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 28       | 0.18          |
| (1,6)   | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 28       | 0.18          |
| (1,6)   | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 28       | 0.18          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H    | 19       | 0.17          |
| (3,17)  | 1:17:A:GLU:O    | 1:20:A:CYS:H    | 16       | 0.17          |
| (3,17)  | 1:17:A:GLU:O    | 1:20:A:CYS:H    | 18       | 0.17          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 4        | 0.17          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 4        | 0.17          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 4        | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 23       | 0.17          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 23       | 0.17          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 23       | 0.17          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG11 | 30       | 0.17          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG12 | 30       | 0.17          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG13 | 30       | 0.17          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG21 | 30       | 0.17          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG22 | 30       | 0.17          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG23 | 30       | 0.17          |
| (1,463) | 1:18:A:ASN:HB2  | 1:19:A:TYR:HD1  | 39       | 0.17          |
| (1,463) | 1:18:A:ASN:HB2  | 1:19:A:TYR:HD2  | 39       | 0.17          |
| (1,463) | 1:18:A:ASN:HB3  | 1:19:A:TYR:HD1  | 39       | 0.17          |
| (1,463) | 1:18:A:ASN:HB3  | 1:19:A:TYR:HD2  | 39       | 0.17          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD11 | 6        | 0.17          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD12 | 6        | 0.17          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD13 | 6        | 0.17          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD21 | 6        | 0.17          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD22 | 6        | 0.17          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD23 | 6        | 0.17          |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB2  | 30       | 0.17          |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB3  | 30       | 0.17          |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB2  | 30       | 0.17          |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB3  | 30       | 0.17          |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB2  | 30       | 0.17          |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB3  | 30       | 0.17          |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB2  | 30       | 0.17          |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB3  | 30       | 0.17          |
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB2  | 30       | 0.17          |
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB3  | 30       | 0.17          |
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB2  | 30       | 0.17          |
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB3  | 30       | 0.17          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 14       | 0.17          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 14       | 0.17          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 14       | 0.17          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 30       | 0.17          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 30       | 0.17          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 30       | 0.17          |
| (1,312) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HB2  | 39       | 0.17          |
| (1,312) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HB2  | 39       | 0.17          |
| (1,312) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HB2  | 39       | 0.17          |
| (1,282) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD21 | 27       | 0.17          |
| (1,282) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD22 | 27       | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,282) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD23 | 27       | 0.17          |
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE1  | 32       | 0.17          |
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE2  | 32       | 0.17          |
| (1,118) | 2:33:B:ASN:HA   | 2:34:B:GLN:H    | 36       | 0.17          |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE1  | 29       | 0.17          |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE2  | 29       | 0.17          |
| (1,17)  | 2:48:B:VAL:HG21 | 2:49:B:CYS:H    | 8        | 0.17          |
| (1,17)  | 2:48:B:VAL:HG22 | 2:49:B:CYS:H    | 8        | 0.17          |
| (1,17)  | 2:48:B:VAL:HG23 | 2:49:B:CYS:H    | 8        | 0.17          |
| (1,17)  | 2:48:B:VAL:HG21 | 2:49:B:CYS:H    | 34       | 0.17          |
| (1,17)  | 2:48:B:VAL:HG22 | 2:49:B:CYS:H    | 34       | 0.17          |
| (1,17)  | 2:48:B:VAL:HG23 | 2:49:B:CYS:H    | 34       | 0.17          |
| (3,31)  | 1:1:A:GLY:O     | 1:5:A:GLN:H     | 9        | 0.16          |
| (3,31)  | 1:1:A:GLY:O     | 1:5:A:GLN:H     | 35       | 0.16          |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H    | 14       | 0.16          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H    | 1        | 0.16          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H    | 29       | 0.16          |
| (3,15)  | 2:39:B:SER:O    | 2:43:B:GLU:H    | 32       | 0.16          |
| (3,7)   | 2:43:B:GLU:O    | 2:47:B:LEU:H    | 11       | 0.16          |
| (3,7)   | 2:43:B:GLU:O    | 2:47:B:LEU:H    | 22       | 0.16          |
| (3,3)   | 2:45:B:LEU:O    | 2:49:B:CYS:H    | 15       | 0.16          |
| (3,3)   | 2:45:B:LEU:O    | 2:49:B:CYS:H    | 18       | 0.16          |
| (3,1)   | 2:46:B:TYR:O    | 2:50:B:GLY:H    | 5        | 0.16          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 25       | 0.16          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 25       | 0.16          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 25       | 0.16          |
| (1,537) | 2:49:B:CYS:HB2  | 2:50:B:GLY:H    | 23       | 0.16          |
| (1,537) | 2:49:B:CYS:HB3  | 2:50:B:GLY:H    | 23       | 0.16          |
| (1,537) | 2:49:B:CYS:HB2  | 2:50:B:GLY:H    | 25       | 0.16          |
| (1,537) | 2:49:B:CYS:HB3  | 2:50:B:GLY:H    | 25       | 0.16          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB2  | 16       | 0.16          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB3  | 16       | 0.16          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB2  | 16       | 0.16          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB3  | 16       | 0.16          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB2  | 16       | 0.16          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB3  | 16       | 0.16          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB2  | 16       | 0.16          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB3  | 16       | 0.16          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB2  | 16       | 0.16          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB3  | 16       | 0.16          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB2  | 16       | 0.16          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB3  | 16       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,472) | 2:31:B:PHE:HD1  | 2:48:B:VAL:HG11 | 35       | 0.16          |
| (1,472) | 2:31:B:PHE:HD1  | 2:48:B:VAL:HG12 | 35       | 0.16          |
| (1,472) | 2:31:B:PHE:HD1  | 2:48:B:VAL:HG13 | 35       | 0.16          |
| (1,472) | 2:31:B:PHE:HD1  | 2:48:B:VAL:HG21 | 35       | 0.16          |
| (1,472) | 2:31:B:PHE:HD1  | 2:48:B:VAL:HG22 | 35       | 0.16          |
| (1,472) | 2:31:B:PHE:HD1  | 2:48:B:VAL:HG23 | 35       | 0.16          |
| (1,472) | 2:31:B:PHE:HD2  | 2:48:B:VAL:HG11 | 35       | 0.16          |
| (1,472) | 2:31:B:PHE:HD2  | 2:48:B:VAL:HG12 | 35       | 0.16          |
| (1,472) | 2:31:B:PHE:HD2  | 2:48:B:VAL:HG13 | 35       | 0.16          |
| (1,472) | 2:31:B:PHE:HD2  | 2:48:B:VAL:HG21 | 35       | 0.16          |
| (1,472) | 2:31:B:PHE:HD2  | 2:48:B:VAL:HG22 | 35       | 0.16          |
| (1,472) | 2:31:B:PHE:HD2  | 2:48:B:VAL:HG23 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 35       | 0.16          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 35       | 0.16          |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB2  | 13       | 0.16          |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB3  | 13       | 0.16          |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB2  | 13       | 0.16          |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB3  | 13       | 0.16          |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB2  | 13       | 0.16          |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB3  | 13       | 0.16          |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB2  | 13       | 0.16          |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB3  | 13       | 0.16          |
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB2  | 13       | 0.16          |
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB3  | 13       | 0.16          |
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB2  | 13       | 0.16          |
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB3  | 13       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,375) | 2:45:B:LEU:HA   | 2:48:B:VAL:HB   | 27       | 0.16          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 16       | 0.16          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 16       | 0.16          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 16       | 0.16          |
| (1,330) | 2:45:B:LEU:HB2  | 2:54:B:PHE:HE1  | 38       | 0.16          |
| (1,330) | 2:45:B:LEU:HB2  | 2:54:B:PHE:HE2  | 38       | 0.16          |
| (1,301) | 1:10:A:ILE:HD11 | 2:33:B:ASN:HB2  | 30       | 0.16          |
| (1,301) | 1:10:A:ILE:HD11 | 2:33:B:ASN:HB3  | 30       | 0.16          |
| (1,301) | 1:10:A:ILE:HD12 | 2:33:B:ASN:HB2  | 30       | 0.16          |
| (1,301) | 1:10:A:ILE:HD12 | 2:33:B:ASN:HB3  | 30       | 0.16          |
| (1,301) | 1:10:A:ILE:HD13 | 2:33:B:ASN:HB2  | 30       | 0.16          |
| (1,301) | 1:10:A:ILE:HD13 | 2:33:B:ASN:HB3  | 30       | 0.16          |
| (1,301) | 1:10:A:ILE:HD11 | 2:33:B:ASN:HB2  | 35       | 0.16          |
| (1,301) | 1:10:A:ILE:HD11 | 2:33:B:ASN:HB3  | 35       | 0.16          |
| (1,301) | 1:10:A:ILE:HD12 | 2:33:B:ASN:HB2  | 35       | 0.16          |
| (1,301) | 1:10:A:ILE:HD12 | 2:33:B:ASN:HB3  | 35       | 0.16          |
| (1,301) | 1:10:A:ILE:HD13 | 2:33:B:ASN:HB2  | 35       | 0.16          |
| (1,301) | 1:10:A:ILE:HD13 | 2:33:B:ASN:HB3  | 35       | 0.16          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG21 | 24       | 0.16          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG22 | 24       | 0.16          |
| (1,246) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG23 | 24       | 0.16          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG21 | 24       | 0.16          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG22 | 24       | 0.16          |
| (1,246) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG23 | 24       | 0.16          |
| (1,234) | 1:14:A:TYR:HA   | 1:14:A:TYR:HE1  | 39       | 0.16          |
| (1,234) | 1:14:A:TYR:HA   | 1:14:A:TYR:HE2  | 39       | 0.16          |
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE1  | 9        | 0.16          |
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE2  | 9        | 0.16          |
| (1,209) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HD1  | 11       | 0.16          |
| (1,209) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HD2  | 11       | 0.16          |
| (1,209) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HD1  | 11       | 0.16          |
| (1,209) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HD2  | 11       | 0.16          |
| (1,209) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HD1  | 11       | 0.16          |
| (1,209) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HD2  | 11       | 0.16          |
| (1,189) | 2:46:B:TYR:H    | 2:54:B:PHE:HE1  | 31       | 0.16          |
| (1,189) | 2:46:B:TYR:H    | 2:54:B:PHE:HE2  | 31       | 0.16          |
| (1,163) | 2:46:B:TYR:HA   | 2:46:B:TYR:HE1  | 14       | 0.16          |
| (1,163) | 2:46:B:TYR:HA   | 2:46:B:TYR:HE2  | 14       | 0.16          |
| (1,136) | 2:42:B:VAL:HG11 | 2:43:B:GLU:H    | 31       | 0.16          |
| (1,136) | 2:42:B:VAL:HG12 | 2:43:B:GLU:H    | 31       | 0.16          |
| (1,136) | 2:42:B:VAL:HG13 | 2:43:B:GLU:H    | 31       | 0.16          |
| (1,111) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HD1  | 6        | 0.16          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,111) | 1:13:A:LEU:HD11 | 2:31:B:PHE:HD2 | 6        | 0.16          |
| (1,111) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HD1 | 6        | 0.16          |
| (1,111) | 1:13:A:LEU:HD12 | 2:31:B:PHE:HD2 | 6        | 0.16          |
| (1,111) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HD1 | 6        | 0.16          |
| (1,111) | 1:13:A:LEU:HD13 | 2:31:B:PHE:HD2 | 6        | 0.16          |
| (1,104) | 1:20:A:CYS:HA   | 1:21:A:ASN:H   | 13       | 0.16          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE1 | 33       | 0.16          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE2 | 33       | 0.16          |
| (1,17)  | 2:48:B:VAL:HG21 | 2:49:B:CYS:H   | 15       | 0.16          |
| (1,17)  | 2:48:B:VAL:HG22 | 2:49:B:CYS:H   | 15       | 0.16          |
| (1,17)  | 2:48:B:VAL:HG23 | 2:49:B:CYS:H   | 15       | 0.16          |
| (1,12)  | 1:10:A:ILE:HD11 | 2:34:B:GLN:H   | 29       | 0.16          |
| (1,12)  | 1:10:A:ILE:HD12 | 2:34:B:GLN:H   | 29       | 0.16          |
| (1,12)  | 1:10:A:ILE:HD13 | 2:34:B:GLN:H   | 29       | 0.16          |
| (1,6)   | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1 | 14       | 0.16          |
| (1,6)   | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1 | 14       | 0.16          |
| (1,6)   | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1 | 14       | 0.16          |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H   | 24       | 0.15          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H   | 20       | 0.15          |
| (3,17)  | 1:17:A:GLU:O    | 1:20:A:CYS:H   | 17       | 0.15          |
| (3,17)  | 1:17:A:GLU:O    | 1:20:A:CYS:H   | 27       | 0.15          |
| (3,6)   | 2:44:B:ALA:O    | 2:48:B:VAL:N   | 27       | 0.15          |
| (3,5)   | 2:44:B:ALA:O    | 2:48:B:VAL:H   | 34       | 0.15          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1 | 13       | 0.15          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1 | 13       | 0.15          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1 | 13       | 0.15          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1 | 35       | 0.15          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1 | 35       | 0.15          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1 | 35       | 0.15          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB2 | 8        | 0.15          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB3 | 8        | 0.15          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB2 | 8        | 0.15          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB3 | 8        | 0.15          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB2 | 8        | 0.15          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB3 | 8        | 0.15          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB2 | 8        | 0.15          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB3 | 8        | 0.15          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB2 | 8        | 0.15          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB3 | 8        | 0.15          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB2 | 8        | 0.15          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB3 | 8        | 0.15          |
| (1,493) | 2:39:B:SER:HB2  | 2:40:B:HIS:HD2 | 35       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,493) | 2:39:B:SER:HB3  | 2:40:B:HIS:HD2  | 35       | 0.15          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 11       | 0.15          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 11       | 0.15          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 11       | 0.15          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 11       | 0.15          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 11       | 0.15          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 11       | 0.15          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD11 | 8        | 0.15          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD12 | 8        | 0.15          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD13 | 8        | 0.15          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD21 | 8        | 0.15          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD22 | 8        | 0.15          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD23 | 8        | 0.15          |
| (1,433) | 1:15:A:GLN:HA   | 1:18:A:ASN:HD21 | 40       | 0.15          |
| (1,433) | 1:15:A:GLN:HA   | 1:18:A:ASN:HD22 | 40       | 0.15          |
| (1,416) | 1:12:A:SER:HB2  | 1:14:A:TYR:HD1  | 21       | 0.15          |
| (1,416) | 1:12:A:SER:HB2  | 1:14:A:TYR:HD2  | 21       | 0.15          |
| (1,416) | 1:12:A:SER:HB3  | 1:14:A:TYR:HD1  | 21       | 0.15          |
| (1,416) | 1:12:A:SER:HB3  | 1:14:A:TYR:HD2  | 21       | 0.15          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD11 | 21       | 0.15          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD12 | 21       | 0.15          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD13 | 21       | 0.15          |
| (1,365) | 1:12:A:SER:HB3  | 1:13:A:LEU:H    | 31       | 0.15          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 9        | 0.15          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 9        | 0.15          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 9        | 0.15          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 32       | 0.15          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 32       | 0.15          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 32       | 0.15          |
| (1,330) | 2:45:B:LEU:HB2  | 2:54:B:PHE:HE1  | 33       | 0.15          |
| (1,330) | 2:45:B:LEU:HB2  | 2:54:B:PHE:HE2  | 33       | 0.15          |
| (1,327) | 2:43:B:GLU:H    | 2:45:B:LEU:HB2  | 27       | 0.15          |
| (1,324) | 2:50:B:GLY:HA2  | 2:51:B:GLU:HA   | 23       | 0.15          |
| (1,324) | 2:50:B:GLY:HA3  | 2:51:B:GLU:HA   | 23       | 0.15          |
| (1,253) | 2:48:B:VAL:HG21 | 2:49:B:CYS:HA   | 22       | 0.15          |
| (1,253) | 2:48:B:VAL:HG22 | 2:49:B:CYS:HA   | 22       | 0.15          |
| (1,253) | 2:48:B:VAL:HG23 | 2:49:B:CYS:HA   | 22       | 0.15          |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE1  | 6        | 0.15          |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE2  | 6        | 0.15          |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE1  | 6        | 0.15          |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE2  | 6        | 0.15          |
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE1  | 6        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE2  | 6        | 0.15          |
| (1,225) | 2:45:B:LEU:HG   | 2:54:B:PHE:HE1  | 16       | 0.15          |
| (1,225) | 2:45:B:LEU:HG   | 2:54:B:PHE:HE2  | 16       | 0.15          |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD1  | 32       | 0.15          |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD2  | 32       | 0.15          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD1  | 32       | 0.15          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD2  | 32       | 0.15          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD1  | 32       | 0.15          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD2  | 32       | 0.15          |
| (1,187) | 2:46:B:TYR:H    | 2:54:B:PHE:HD1  | 12       | 0.15          |
| (1,187) | 2:46:B:TYR:H    | 2:54:B:PHE:HD2  | 12       | 0.15          |
| (1,127) | 2:37:B:CYS:H    | 2:40:B:HIS:HB3  | 40       | 0.15          |
| (1,18)  | 2:48:B:VAL:HG11 | 2:49:B:CYS:H    | 24       | 0.15          |
| (1,18)  | 2:48:B:VAL:HG12 | 2:49:B:CYS:H    | 24       | 0.15          |
| (1,18)  | 2:48:B:VAL:HG13 | 2:49:B:CYS:H    | 24       | 0.15          |
| (1,17)  | 2:48:B:VAL:HG21 | 2:49:B:CYS:H    | 21       | 0.15          |
| (1,17)  | 2:48:B:VAL:HG22 | 2:49:B:CYS:H    | 21       | 0.15          |
| (1,17)  | 2:48:B:VAL:HG23 | 2:49:B:CYS:H    | 21       | 0.15          |
| (1,13)  | 2:32:B:VAL:HG11 | 2:33:B:ASN:H    | 7        | 0.15          |
| (1,13)  | 2:32:B:VAL:HG12 | 2:33:B:ASN:H    | 7        | 0.15          |
| (1,13)  | 2:32:B:VAL:HG13 | 2:33:B:ASN:H    | 7        | 0.15          |
| (1,13)  | 2:32:B:VAL:HG21 | 2:33:B:ASN:H    | 7        | 0.15          |
| (1,13)  | 2:32:B:VAL:HG22 | 2:33:B:ASN:H    | 7        | 0.15          |
| (1,13)  | 2:32:B:VAL:HG23 | 2:33:B:ASN:H    | 7        | 0.15          |
| (1,6)   | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 15       | 0.15          |
| (1,6)   | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 15       | 0.15          |
| (1,6)   | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 15       | 0.15          |
| (3,31)  | 1:1:A:GLY:O     | 1:5:A:GLN:H     | 32       | 0.14          |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H    | 8        | 0.14          |
| (3,20)  | 1:16:A:LEU:O    | 1:19:A:TYR:N    | 11       | 0.14          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H    | 17       | 0.14          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H    | 39       | 0.14          |
| (3,15)  | 2:39:B:SER:O    | 2:43:B:GLU:H    | 23       | 0.14          |
| (3,11)  | 2:41:B:LEU:O    | 2:45:B:LEU:H    | 38       | 0.14          |
| (3,9)   | 2:42:B:VAL:O    | 2:46:B:TYR:H    | 35       | 0.14          |
| (3,4)   | 2:45:B:LEU:O    | 2:49:B:CYS:N    | 18       | 0.14          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 27       | 0.14          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 27       | 0.14          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 27       | 0.14          |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG11 | 21       | 0.14          |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG12 | 21       | 0.14          |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG13 | 21       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG21 | 21       | 0.14          |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG22 | 21       | 0.14          |
| (1,520) | 2:45:B:LEU:HB2  | 2:48:B:VAL:HG23 | 21       | 0.14          |
| (1,511) | 2:42:B:VAL:HG11 | 2:54:B:PHE:HE1  | 35       | 0.14          |
| (1,511) | 2:42:B:VAL:HG11 | 2:54:B:PHE:HE2  | 35       | 0.14          |
| (1,511) | 2:42:B:VAL:HG12 | 2:54:B:PHE:HE1  | 35       | 0.14          |
| (1,511) | 2:42:B:VAL:HG12 | 2:54:B:PHE:HE2  | 35       | 0.14          |
| (1,511) | 2:42:B:VAL:HG13 | 2:54:B:PHE:HE1  | 35       | 0.14          |
| (1,511) | 2:42:B:VAL:HG13 | 2:54:B:PHE:HE2  | 35       | 0.14          |
| (1,511) | 2:42:B:VAL:HG21 | 2:54:B:PHE:HE1  | 35       | 0.14          |
| (1,511) | 2:42:B:VAL:HG21 | 2:54:B:PHE:HE2  | 35       | 0.14          |
| (1,511) | 2:42:B:VAL:HG22 | 2:54:B:PHE:HE1  | 35       | 0.14          |
| (1,511) | 2:42:B:VAL:HG22 | 2:54:B:PHE:HE2  | 35       | 0.14          |
| (1,511) | 2:42:B:VAL:HG23 | 2:54:B:PHE:HE1  | 35       | 0.14          |
| (1,511) | 2:42:B:VAL:HG23 | 2:54:B:PHE:HE2  | 35       | 0.14          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD11 | 10       | 0.14          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD12 | 10       | 0.14          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD13 | 10       | 0.14          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD21 | 10       | 0.14          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD22 | 10       | 0.14          |
| (1,500) | 2:41:B:LEU:HG   | 2:45:B:LEU:HD23 | 10       | 0.14          |
| (1,483) | 2:36:B:LEU:HB2  | 2:40:B:HIS:HB2  | 20       | 0.14          |
| (1,483) | 2:36:B:LEU:HB2  | 2:40:B:HIS:HB3  | 20       | 0.14          |
| (1,483) | 2:36:B:LEU:HB3  | 2:40:B:HIS:HB2  | 20       | 0.14          |
| (1,483) | 2:36:B:LEU:HB3  | 2:40:B:HIS:HB3  | 20       | 0.14          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD11 | 24       | 0.14          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD12 | 24       | 0.14          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD13 | 24       | 0.14          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD21 | 24       | 0.14          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD22 | 24       | 0.14          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD23 | 24       | 0.14          |
| (1,413) | 1:12:A:SER:HA   | 1:13:A:LEU:HB2  | 40       | 0.14          |
| (1,413) | 1:12:A:SER:HA   | 1:13:A:LEU:HB3  | 40       | 0.14          |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB2  | 1        | 0.14          |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB3  | 1        | 0.14          |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB2  | 1        | 0.14          |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB3  | 1        | 0.14          |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB2  | 1        | 0.14          |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB3  | 1        | 0.14          |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB2  | 1        | 0.14          |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB3  | 1        | 0.14          |
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB2  | 1        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB3  | 1        | 0.14          |
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB2  | 1        | 0.14          |
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB3  | 1        | 0.14          |
| (1,377) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD11 | 17       | 0.14          |
| (1,377) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD12 | 17       | 0.14          |
| (1,377) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD13 | 17       | 0.14          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD11 | 20       | 0.14          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD12 | 20       | 0.14          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD13 | 20       | 0.14          |
| (1,352) | 1:4:A:GLU:HA    | 1:8:A:THR:HG21  | 36       | 0.14          |
| (1,352) | 1:4:A:GLU:HA    | 1:8:A:THR:HG22  | 36       | 0.14          |
| (1,352) | 1:4:A:GLU:HA    | 1:8:A:THR:HG23  | 36       | 0.14          |
| (1,347) | 2:32:B:VAL:HA   | 2:33:B:ASN:HB2  | 7        | 0.14          |
| (1,347) | 2:32:B:VAL:HA   | 2:33:B:ASN:HB3  | 7        | 0.14          |
| (1,338) | 2:42:B:VAL:HB   | 2:54:B:PHE:HE1  | 10       | 0.14          |
| (1,338) | 2:42:B:VAL:HB   | 2:54:B:PHE:HE2  | 10       | 0.14          |
| (1,338) | 2:42:B:VAL:HB   | 2:54:B:PHE:HE1  | 15       | 0.14          |
| (1,338) | 2:42:B:VAL:HB   | 2:54:B:PHE:HE2  | 15       | 0.14          |
| (1,337) | 1:16:A:LEU:HG   | 1:19:A:TYR:HE1  | 18       | 0.14          |
| (1,337) | 1:16:A:LEU:HG   | 1:19:A:TYR:HE2  | 18       | 0.14          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG11 | 2        | 0.14          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG12 | 2        | 0.14          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG13 | 2        | 0.14          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG21 | 2        | 0.14          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG22 | 2        | 0.14          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG23 | 2        | 0.14          |
| (1,327) | 2:43:B:GLU:H    | 2:45:B:LEU:HB2  | 15       | 0.14          |
| (1,282) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD21 | 30       | 0.14          |
| (1,282) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD22 | 30       | 0.14          |
| (1,282) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD23 | 30       | 0.14          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG21 | 35       | 0.14          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG22 | 35       | 0.14          |
| (1,276) | 1:17:A:GLU:HA   | 2:48:B:VAL:HG23 | 35       | 0.14          |
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE1  | 19       | 0.14          |
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE2  | 19       | 0.14          |
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE1  | 25       | 0.14          |
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE2  | 25       | 0.14          |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE1  | 19       | 0.14          |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE2  | 19       | 0.14          |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE1  | 19       | 0.14          |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE2  | 19       | 0.14          |
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE1  | 19       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE2  | 19       | 0.14          |
| (1,225) | 2:45:B:LEU:HG   | 2:54:B:PHE:HE1  | 4        | 0.14          |
| (1,225) | 2:45:B:LEU:HG   | 2:54:B:PHE:HE2  | 4        | 0.14          |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD1  | 18       | 0.14          |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD2  | 18       | 0.14          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD1  | 18       | 0.14          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD2  | 18       | 0.14          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD1  | 18       | 0.14          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD2  | 18       | 0.14          |
| (1,191) | 2:54:B:PHE:HA   | 2:55:B:PHE:H    | 15       | 0.14          |
| (1,191) | 2:54:B:PHE:HA   | 2:55:B:PHE:H    | 20       | 0.14          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD11 | 40       | 0.14          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD12 | 40       | 0.14          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD13 | 40       | 0.14          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD21 | 40       | 0.14          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD22 | 40       | 0.14          |
| (1,166) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HD23 | 40       | 0.14          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD11 | 40       | 0.14          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD12 | 40       | 0.14          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD13 | 40       | 0.14          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD21 | 40       | 0.14          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD22 | 40       | 0.14          |
| (1,166) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HD23 | 40       | 0.14          |
| (1,136) | 2:42:B:VAL:HG11 | 2:43:B:GLU:H    | 8        | 0.14          |
| (1,136) | 2:42:B:VAL:HG12 | 2:43:B:GLU:H    | 8        | 0.14          |
| (1,136) | 2:42:B:VAL:HG13 | 2:43:B:GLU:H    | 8        | 0.14          |
| (1,104) | 1:20:A:CYS:HA   | 1:21:A:ASN:H    | 20       | 0.14          |
| (1,17)  | 2:48:B:VAL:HG21 | 2:49:B:CYS:H    | 2        | 0.14          |
| (1,17)  | 2:48:B:VAL:HG22 | 2:49:B:CYS:H    | 2        | 0.14          |
| (1,17)  | 2:48:B:VAL:HG23 | 2:49:B:CYS:H    | 2        | 0.14          |
| (1,17)  | 2:48:B:VAL:HG21 | 2:49:B:CYS:H    | 14       | 0.14          |
| (1,17)  | 2:48:B:VAL:HG22 | 2:49:B:CYS:H    | 14       | 0.14          |
| (1,17)  | 2:48:B:VAL:HG23 | 2:49:B:CYS:H    | 14       | 0.14          |
| (1,6)   | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 21       | 0.14          |
| (1,6)   | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 21       | 0.14          |
| (1,6)   | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 21       | 0.14          |
| (1,6)   | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 37       | 0.14          |
| (1,6)   | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 37       | 0.14          |
| (1,6)   | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 37       | 0.14          |
| (3,25)  | 1:12:A:SER:O    | 1:16:A:LEU:H    | 30       | 0.13          |
| (3,20)  | 1:16:A:LEU:O    | 1:19:A:TYR:N    | 6        | 0.13          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H    | 35       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H    | 40       | 0.13          |
| (3,17)  | 1:17:A:GLU:O    | 1:20:A:CYS:H    | 14       | 0.13          |
| (3,17)  | 1:17:A:GLU:O    | 1:20:A:CYS:H    | 34       | 0.13          |
| (3,17)  | 1:17:A:GLU:O    | 1:20:A:CYS:H    | 40       | 0.13          |
| (3,11)  | 2:41:B:LEU:O    | 2:45:B:LEU:H    | 21       | 0.13          |
| (3,7)   | 2:43:B:GLU:O    | 2:47:B:LEU:H    | 37       | 0.13          |
| (3,3)   | 2:45:B:LEU:O    | 2:49:B:CYS:H    | 20       | 0.13          |
| (3,3)   | 2:45:B:LEU:O    | 2:49:B:CYS:H    | 36       | 0.13          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 12       | 0.13          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 12       | 0.13          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 12       | 0.13          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 26       | 0.13          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 26       | 0.13          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 26       | 0.13          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE1  | 7        | 0.13          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE2  | 7        | 0.13          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE1  | 7        | 0.13          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE2  | 7        | 0.13          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE1  | 7        | 0.13          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE2  | 7        | 0.13          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE1  | 7        | 0.13          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE2  | 7        | 0.13          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE1  | 7        | 0.13          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE2  | 7        | 0.13          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE1  | 7        | 0.13          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE2  | 7        | 0.13          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG11 | 18       | 0.13          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG12 | 18       | 0.13          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG13 | 18       | 0.13          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG21 | 18       | 0.13          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG22 | 18       | 0.13          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG23 | 18       | 0.13          |
| (1,493) | 2:39:B:SER:HB2  | 2:40:B:HIS:HD2  | 29       | 0.13          |
| (1,493) | 2:39:B:SER:HB3  | 2:40:B:HIS:HD2  | 29       | 0.13          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG11 | 2        | 0.13          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG12 | 2        | 0.13          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG13 | 2        | 0.13          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG21 | 2        | 0.13          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG22 | 2        | 0.13          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG23 | 2        | 0.13          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG11 | 12       | 0.13          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG12 | 12       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG13 | 12       | 0.13          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG21 | 12       | 0.13          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG22 | 12       | 0.13          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG23 | 12       | 0.13          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD11 | 32       | 0.13          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD12 | 32       | 0.13          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD13 | 32       | 0.13          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 35       | 0.13          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 35       | 0.13          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 35       | 0.13          |
| (1,326) | 2:43:B:GLU:H    | 2:45:B:LEU:HB3  | 19       | 0.13          |
| (1,233) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HA   | 24       | 0.13          |
| (1,233) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HA   | 24       | 0.13          |
| (1,225) | 2:45:B:LEU:HG   | 2:54:B:PHE:HE1  | 39       | 0.13          |
| (1,225) | 2:45:B:LEU:HG   | 2:54:B:PHE:HE2  | 39       | 0.13          |
| (1,209) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HD1  | 33       | 0.13          |
| (1,209) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HD2  | 33       | 0.13          |
| (1,209) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HD1  | 33       | 0.13          |
| (1,209) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HD2  | 33       | 0.13          |
| (1,209) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HD1  | 33       | 0.13          |
| (1,209) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HD2  | 33       | 0.13          |
| (1,142) | 2:42:B:VAL:HB   | 2:43:B:GLU:H    | 12       | 0.13          |
| (1,6)   | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 1        | 0.13          |
| (1,6)   | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 1        | 0.13          |
| (1,6)   | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 1        | 0.13          |
| (1,5)   | 1:10:A:ILE:HD11 | 2:35:B:HIS:HE1  | 40       | 0.13          |
| (1,5)   | 1:10:A:ILE:HD12 | 2:35:B:HIS:HE1  | 40       | 0.13          |
| (1,5)   | 1:10:A:ILE:HD13 | 2:35:B:HIS:HE1  | 40       | 0.13          |
| (3,31)  | 1:1:A:GLY:O     | 1:5:A:GLN:H     | 1        | 0.12          |
| (3,31)  | 1:1:A:GLY:O     | 1:5:A:GLN:H     | 34       | 0.12          |
| (3,29)  | 1:2:A:ILE:O     | 1:6:A:CYS:H     | 11       | 0.12          |
| (3,27)  | 1:3:A:VAL:O     | 1:7:A:CYS:H     | 17       | 0.12          |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H    | 15       | 0.12          |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H    | 31       | 0.12          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H    | 23       | 0.12          |
| (3,18)  | 1:17:A:GLU:O    | 1:20:A:CYS:N    | 30       | 0.12          |
| (3,17)  | 1:17:A:GLU:O    | 1:20:A:CYS:H    | 35       | 0.12          |
| (3,15)  | 2:39:B:SER:O    | 2:43:B:GLU:H    | 27       | 0.12          |
| (3,15)  | 2:39:B:SER:O    | 2:43:B:GLU:H    | 36       | 0.12          |
| (3,13)  | 2:40:B:HIS:O    | 2:44:B:ALA:H    | 31       | 0.12          |
| (3,12)  | 2:41:B:LEU:O    | 2:45:B:LEU:N    | 38       | 0.12          |
| (3,11)  | 2:41:B:LEU:O    | 2:45:B:LEU:H    | 6        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,11)  | 2:41:B:LEU:O    | 2:45:B:LEU:H    | 34       | 0.12          |
| (3,6)   | 2:44:B:ALA:O    | 2:48:B:VAL:N    | 34       | 0.12          |
| (3,5)   | 2:44:B:ALA:O    | 2:48:B:VAL:H    | 15       | 0.12          |
| (3,5)   | 2:44:B:ALA:O    | 2:48:B:VAL:H    | 22       | 0.12          |
| (3,1)   | 2:46:B:TYR:O    | 2:50:B:GLY:H    | 25       | 0.12          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 2        | 0.12          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 2        | 0.12          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 2        | 0.12          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 38       | 0.12          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 38       | 0.12          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 38       | 0.12          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE1  | 1        | 0.12          |
| (1,535) | 2:48:B:VAL:HG11 | 2:54:B:PHE:HE2  | 1        | 0.12          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE1  | 1        | 0.12          |
| (1,535) | 2:48:B:VAL:HG12 | 2:54:B:PHE:HE2  | 1        | 0.12          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE1  | 1        | 0.12          |
| (1,535) | 2:48:B:VAL:HG13 | 2:54:B:PHE:HE2  | 1        | 0.12          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE1  | 1        | 0.12          |
| (1,535) | 2:48:B:VAL:HG21 | 2:54:B:PHE:HE2  | 1        | 0.12          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE1  | 1        | 0.12          |
| (1,535) | 2:48:B:VAL:HG22 | 2:54:B:PHE:HE2  | 1        | 0.12          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE1  | 1        | 0.12          |
| (1,535) | 2:48:B:VAL:HG23 | 2:54:B:PHE:HE2  | 1        | 0.12          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB2  | 17       | 0.12          |
| (1,523) | 2:45:B:LEU:HD11 | 2:54:B:PHE:HB3  | 17       | 0.12          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB2  | 17       | 0.12          |
| (1,523) | 2:45:B:LEU:HD12 | 2:54:B:PHE:HB3  | 17       | 0.12          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB2  | 17       | 0.12          |
| (1,523) | 2:45:B:LEU:HD13 | 2:54:B:PHE:HB3  | 17       | 0.12          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB2  | 17       | 0.12          |
| (1,523) | 2:45:B:LEU:HD21 | 2:54:B:PHE:HB3  | 17       | 0.12          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB2  | 17       | 0.12          |
| (1,523) | 2:45:B:LEU:HD22 | 2:54:B:PHE:HB3  | 17       | 0.12          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB2  | 17       | 0.12          |
| (1,523) | 2:45:B:LEU:HD23 | 2:54:B:PHE:HB3  | 17       | 0.12          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG11 | 10       | 0.12          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG12 | 10       | 0.12          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG13 | 10       | 0.12          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG21 | 10       | 0.12          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG22 | 10       | 0.12          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG23 | 10       | 0.12          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 26       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 26       | 0.12          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 26       | 0.12          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 26       | 0.12          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 26       | 0.12          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 26       | 0.12          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 16       | 0.12          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 16       | 0.12          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD11 | 6        | 0.12          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD12 | 6        | 0.12          |
| (1,376) | 1:13:A:LEU:HA   | 1:16:A:LEU:HD13 | 6        | 0.12          |
| (1,375) | 2:45:B:LEU:HA   | 2:48:B:VAL:HB   | 13       | 0.12          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 6        | 0.12          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 6        | 0.12          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 6        | 0.12          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 11       | 0.12          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 11       | 0.12          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 11       | 0.12          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 17       | 0.12          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 17       | 0.12          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 17       | 0.12          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 29       | 0.12          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 29       | 0.12          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 29       | 0.12          |
| (1,344) | 2:32:B:VAL:HG11 | 2:34:B:GLN:H    | 13       | 0.12          |
| (1,344) | 2:32:B:VAL:HG12 | 2:34:B:GLN:H    | 13       | 0.12          |
| (1,344) | 2:32:B:VAL:HG13 | 2:34:B:GLN:H    | 13       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,344) | 2:32:B:VAL:HG21 | 2:34:B:GLN:H    | 13       | 0.12          |
| (1,344) | 2:32:B:VAL:HG22 | 2:34:B:GLN:H    | 13       | 0.12          |
| (1,344) | 2:32:B:VAL:HG23 | 2:34:B:GLN:H    | 13       | 0.12          |
| (1,338) | 2:42:B:VAL:HB   | 2:54:B:PHE:HE1  | 14       | 0.12          |
| (1,338) | 2:42:B:VAL:HB   | 2:54:B:PHE:HE2  | 14       | 0.12          |
| (1,338) | 2:42:B:VAL:HB   | 2:54:B:PHE:HE1  | 20       | 0.12          |
| (1,338) | 2:42:B:VAL:HB   | 2:54:B:PHE:HE2  | 20       | 0.12          |
| (1,299) | 1:6:A:CYS:HB3   | 2:41:B:LEU:HD21 | 28       | 0.12          |
| (1,299) | 1:6:A:CYS:HB3   | 2:41:B:LEU:HD22 | 28       | 0.12          |
| (1,299) | 1:6:A:CYS:HB3   | 2:41:B:LEU:HD23 | 28       | 0.12          |
| (1,254) | 2:48:B:VAL:HG11 | 2:49:B:CYS:HA   | 31       | 0.12          |
| (1,254) | 2:48:B:VAL:HG12 | 2:49:B:CYS:HA   | 31       | 0.12          |
| (1,254) | 2:48:B:VAL:HG13 | 2:49:B:CYS:HA   | 31       | 0.12          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG11 | 21       | 0.12          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG12 | 21       | 0.12          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG13 | 21       | 0.12          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG11 | 21       | 0.12          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG12 | 21       | 0.12          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG13 | 21       | 0.12          |
| (1,242) | 2:54:B:PHE:H    | 2:54:B:PHE:HE1  | 8        | 0.12          |
| (1,242) | 2:54:B:PHE:H    | 2:54:B:PHE:HE2  | 8        | 0.12          |
| (1,242) | 2:54:B:PHE:H    | 2:54:B:PHE:HE1  | 40       | 0.12          |
| (1,242) | 2:54:B:PHE:H    | 2:54:B:PHE:HE2  | 40       | 0.12          |
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE1  | 10       | 0.12          |
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE2  | 10       | 0.12          |
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE1  | 20       | 0.12          |
| (1,229) | 1:2:A:ILE:HG12  | 1:19:A:TYR:HE2  | 20       | 0.12          |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE1  | 34       | 0.12          |
| (1,227) | 1:2:A:ILE:HG21  | 1:19:A:TYR:HE2  | 34       | 0.12          |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE1  | 34       | 0.12          |
| (1,227) | 1:2:A:ILE:HG22  | 1:19:A:TYR:HE2  | 34       | 0.12          |
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE1  | 34       | 0.12          |
| (1,227) | 1:2:A:ILE:HG23  | 1:19:A:TYR:HE2  | 34       | 0.12          |
| (1,219) | 2:59:B:LYS:HA   | 2:60:B:THR:H    | 22       | 0.12          |
| (1,218) | 2:58:B:PRO:HG2  | 2:59:B:LYS:H    | 14       | 0.12          |
| (1,218) | 2:58:B:PRO:HG3  | 2:59:B:LYS:H    | 14       | 0.12          |
| (1,211) | 1:19:A:TYR:HD1  | 2:45:B:LEU:HD21 | 24       | 0.12          |
| (1,211) | 1:19:A:TYR:HD1  | 2:45:B:LEU:HD22 | 24       | 0.12          |
| (1,211) | 1:19:A:TYR:HD1  | 2:45:B:LEU:HD23 | 24       | 0.12          |
| (1,211) | 1:19:A:TYR:HD2  | 2:45:B:LEU:HD21 | 24       | 0.12          |
| (1,211) | 1:19:A:TYR:HD2  | 2:45:B:LEU:HD22 | 24       | 0.12          |
| (1,211) | 1:19:A:TYR:HD2  | 2:45:B:LEU:HD23 | 24       | 0.12          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD1 | 5        | 0.12          |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD2 | 5        | 0.12          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD1 | 5        | 0.12          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD2 | 5        | 0.12          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD1 | 5        | 0.12          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD2 | 5        | 0.12          |
| (1,180) | 2:52:B:GLN:H    | 2:53:B:GLY:H   | 34       | 0.12          |
| (1,127) | 2:37:B:CYS:H    | 2:40:B:HIS:HB3 | 36       | 0.12          |
| (1,110) | 1:13:A:LEU:HD21 | 2:31:B:PHE:HD1 | 5        | 0.12          |
| (1,110) | 1:13:A:LEU:HD21 | 2:31:B:PHE:HD2 | 5        | 0.12          |
| (1,110) | 1:13:A:LEU:HD22 | 2:31:B:PHE:HD1 | 5        | 0.12          |
| (1,110) | 1:13:A:LEU:HD22 | 2:31:B:PHE:HD2 | 5        | 0.12          |
| (1,110) | 1:13:A:LEU:HD23 | 2:31:B:PHE:HD1 | 5        | 0.12          |
| (1,110) | 1:13:A:LEU:HD23 | 2:31:B:PHE:HD2 | 5        | 0.12          |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE1 | 10       | 0.12          |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE2 | 10       | 0.12          |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE1 | 39       | 0.12          |
| (1,45)  | 1:2:A:ILE:H     | 1:19:A:TYR:HE2 | 39       | 0.12          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE1 | 14       | 0.12          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE2 | 14       | 0.12          |
| (1,17)  | 2:48:B:VAL:HG21 | 2:49:B:CYS:H   | 35       | 0.12          |
| (1,17)  | 2:48:B:VAL:HG22 | 2:49:B:CYS:H   | 35       | 0.12          |
| (1,17)  | 2:48:B:VAL:HG23 | 2:49:B:CYS:H   | 35       | 0.12          |
| (1,5)   | 1:10:A:ILE:HD11 | 2:35:B:HIS:HE1 | 15       | 0.12          |
| (1,5)   | 1:10:A:ILE:HD12 | 2:35:B:HIS:HE1 | 15       | 0.12          |
| (1,5)   | 1:10:A:ILE:HD13 | 2:35:B:HIS:HE1 | 15       | 0.12          |
| (3,31)  | 1:1:A:GLY:O     | 1:5:A:GLN:H    | 22       | 0.11          |
| (3,27)  | 1:3:A:VAL:O     | 1:7:A:CYS:H    | 38       | 0.11          |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H   | 6        | 0.11          |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H   | 29       | 0.11          |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H   | 33       | 0.11          |
| (3,20)  | 1:16:A:LEU:O    | 1:19:A:TYR:N   | 20       | 0.11          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H   | 21       | 0.11          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H   | 31       | 0.11          |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H   | 34       | 0.11          |
| (3,17)  | 1:17:A:GLU:O    | 1:20:A:CYS:H   | 10       | 0.11          |
| (3,13)  | 2:40:B:HIS:O    | 2:44:B:ALA:H   | 6        | 0.11          |
| (3,11)  | 2:41:B:LEU:O    | 2:45:B:LEU:H   | 24       | 0.11          |
| (3,7)   | 2:43:B:GLU:O    | 2:47:B:LEU:H   | 24       | 0.11          |
| (3,7)   | 2:43:B:GLU:O    | 2:47:B:LEU:H   | 35       | 0.11          |
| (3,5)   | 2:44:B:ALA:O    | 2:48:B:VAL:H   | 33       | 0.11          |
| (3,3)   | 2:45:B:LEU:O    | 2:49:B:CYS:H   | 13       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,3)   | 2:45:B:LEU:O    | 2:49:B:CYS:H    | 26       | 0.11          |
| (1,557) | 1:10:A:ILE:HG21 | 2:35:B:HIS:HE1  | 5        | 0.11          |
| (1,557) | 1:10:A:ILE:HG22 | 2:35:B:HIS:HE1  | 5        | 0.11          |
| (1,557) | 1:10:A:ILE:HG23 | 2:35:B:HIS:HE1  | 5        | 0.11          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG11 | 14       | 0.11          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG12 | 14       | 0.11          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG13 | 14       | 0.11          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG21 | 14       | 0.11          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG22 | 14       | 0.11          |
| (1,514) | 2:44:B:ALA:HA   | 2:48:B:VAL:HG23 | 14       | 0.11          |
| (1,494) | 2:39:B:SER:HB2  | 2:42:B:VAL:HG11 | 14       | 0.11          |
| (1,494) | 2:39:B:SER:HB2  | 2:42:B:VAL:HG12 | 14       | 0.11          |
| (1,494) | 2:39:B:SER:HB2  | 2:42:B:VAL:HG13 | 14       | 0.11          |
| (1,494) | 2:39:B:SER:HB2  | 2:42:B:VAL:HG21 | 14       | 0.11          |
| (1,494) | 2:39:B:SER:HB2  | 2:42:B:VAL:HG22 | 14       | 0.11          |
| (1,494) | 2:39:B:SER:HB2  | 2:42:B:VAL:HG23 | 14       | 0.11          |
| (1,494) | 2:39:B:SER:HB3  | 2:42:B:VAL:HG11 | 14       | 0.11          |
| (1,494) | 2:39:B:SER:HB3  | 2:42:B:VAL:HG12 | 14       | 0.11          |
| (1,494) | 2:39:B:SER:HB3  | 2:42:B:VAL:HG13 | 14       | 0.11          |
| (1,494) | 2:39:B:SER:HB3  | 2:42:B:VAL:HG21 | 14       | 0.11          |
| (1,494) | 2:39:B:SER:HB3  | 2:42:B:VAL:HG22 | 14       | 0.11          |
| (1,494) | 2:39:B:SER:HB3  | 2:42:B:VAL:HG23 | 14       | 0.11          |
| (1,493) | 2:39:B:SER:HB2  | 2:40:B:HIS:HD2  | 1        | 0.11          |
| (1,493) | 2:39:B:SER:HB3  | 2:40:B:HIS:HD2  | 1        | 0.11          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG11 | 33       | 0.11          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG12 | 33       | 0.11          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG13 | 33       | 0.11          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG21 | 33       | 0.11          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG22 | 33       | 0.11          |
| (1,473) | 2:31:B:PHE:HZ   | 2:48:B:VAL:HG23 | 33       | 0.11          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 9        | 0.11          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 9        | 0.11          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 9        | 0.11          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 9        | 0.11          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 9        | 0.11          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 9        | 0.11          |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG   | 35       | 0.11          |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG   | 35       | 0.11          |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG   | 35       | 0.11          |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG   | 35       | 0.11          |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG   | 35       | 0.11          |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG   | 35       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD11 | 25       | 0.11          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD12 | 25       | 0.11          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD13 | 25       | 0.11          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD21 | 25       | 0.11          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD22 | 25       | 0.11          |
| (1,440) | 1:16:A:LEU:HA   | 2:45:B:LEU:HD23 | 25       | 0.11          |
| (1,422) | 1:13:A:LEU:HB2  | 2:31:B:PHE:HD1  | 19       | 0.11          |
| (1,422) | 1:13:A:LEU:HB2  | 2:31:B:PHE:HD2  | 19       | 0.11          |
| (1,422) | 1:13:A:LEU:HB3  | 2:31:B:PHE:HD1  | 19       | 0.11          |
| (1,422) | 1:13:A:LEU:HB3  | 2:31:B:PHE:HD2  | 19       | 0.11          |
| (1,416) | 1:12:A:SER:HB2  | 1:14:A:TYR:HD1  | 7        | 0.11          |
| (1,416) | 1:12:A:SER:HB2  | 1:14:A:TYR:HD2  | 7        | 0.11          |
| (1,416) | 1:12:A:SER:HB3  | 1:14:A:TYR:HD1  | 7        | 0.11          |
| (1,416) | 1:12:A:SER:HB3  | 1:14:A:TYR:HD2  | 7        | 0.11          |
| (1,393) | 2:31:B:PHE:HZ   | 2:33:B:ASN:HA   | 11       | 0.11          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD11 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD12 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD13 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD21 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD22 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB1  | 2:47:B:LEU:HD23 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD11 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD12 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD13 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD21 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD22 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB2  | 2:47:B:LEU:HD23 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD11 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD12 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD13 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD21 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD22 | 6        | 0.11          |
| (1,387) | 2:44:B:ALA:HB3  | 2:47:B:LEU:HD23 | 6        | 0.11          |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB2  | 8        | 0.11          |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB3  | 8        | 0.11          |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB2  | 8        | 0.11          |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB3  | 8        | 0.11          |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB2  | 8        | 0.11          |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB3  | 8        | 0.11          |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB2  | 8        | 0.11          |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB3  | 8        | 0.11          |
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB2  | 8        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB3  | 8        | 0.11          |
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB2  | 8        | 0.11          |
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB3  | 8        | 0.11          |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB2  | 10       | 0.11          |
| (1,384) | 2:32:B:VAL:HG11 | 2:33:B:ASN:HB3  | 10       | 0.11          |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB2  | 10       | 0.11          |
| (1,384) | 2:32:B:VAL:HG12 | 2:33:B:ASN:HB3  | 10       | 0.11          |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB2  | 10       | 0.11          |
| (1,384) | 2:32:B:VAL:HG13 | 2:33:B:ASN:HB3  | 10       | 0.11          |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB2  | 10       | 0.11          |
| (1,384) | 2:32:B:VAL:HG21 | 2:33:B:ASN:HB3  | 10       | 0.11          |
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB2  | 10       | 0.11          |
| (1,384) | 2:32:B:VAL:HG22 | 2:33:B:ASN:HB3  | 10       | 0.11          |
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB2  | 10       | 0.11          |
| (1,384) | 2:32:B:VAL:HG23 | 2:33:B:ASN:HB3  | 10       | 0.11          |
| (1,377) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD11 | 24       | 0.11          |
| (1,377) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD12 | 24       | 0.11          |
| (1,377) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD13 | 24       | 0.11          |
| (1,354) | 1:4:A:GLU:HG2   | 1:8:A:THR:HG21  | 9        | 0.11          |
| (1,354) | 1:4:A:GLU:HG2   | 1:8:A:THR:HG22  | 9        | 0.11          |
| (1,354) | 1:4:A:GLU:HG2   | 1:8:A:THR:HG23  | 9        | 0.11          |
| (1,354) | 1:4:A:GLU:HG3   | 1:8:A:THR:HG21  | 9        | 0.11          |
| (1,354) | 1:4:A:GLU:HG3   | 1:8:A:THR:HG22  | 9        | 0.11          |
| (1,354) | 1:4:A:GLU:HG3   | 1:8:A:THR:HG23  | 9        | 0.11          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 8        | 0.11          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 8        | 0.11          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 8        | 0.11          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 34       | 0.11          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 34       | 0.11          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 34       | 0.11          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG21 | 38       | 0.11          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG22 | 38       | 0.11          |
| (1,353) | 2:45:B:LEU:HA   | 2:48:B:VAL:HG23 | 38       | 0.11          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG11 | 34       | 0.11          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG12 | 34       | 0.11          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG13 | 34       | 0.11          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG21 | 34       | 0.11          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG22 | 34       | 0.11          |
| (1,328) | 2:31:B:PHE:HZ   | 2:32:B:VAL:HG23 | 34       | 0.11          |
| (1,327) | 2:43:B:GLU:H    | 2:45:B:LEU:HB2  | 11       | 0.11          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD11 | 17       | 0.11          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD12 | 17       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD13 | 17       | 0.11          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD21 | 17       | 0.11          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD22 | 17       | 0.11          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD23 | 17       | 0.11          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD11 | 30       | 0.11          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD12 | 30       | 0.11          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD13 | 30       | 0.11          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD21 | 30       | 0.11          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD22 | 30       | 0.11          |
| (1,303) | 2:34:B:GLN:HG3  | 2:36:B:LEU:HD23 | 30       | 0.11          |
| (1,282) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD21 | 6        | 0.11          |
| (1,282) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD22 | 6        | 0.11          |
| (1,282) | 1:13:A:LEU:HA   | 1:13:A:LEU:HD23 | 6        | 0.11          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG11 | 32       | 0.11          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG12 | 32       | 0.11          |
| (1,247) | 2:31:B:PHE:HE1  | 2:48:B:VAL:HG13 | 32       | 0.11          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG11 | 32       | 0.11          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG12 | 32       | 0.11          |
| (1,247) | 2:31:B:PHE:HE2  | 2:48:B:VAL:HG13 | 32       | 0.11          |
| (1,233) | 2:46:B:TYR:HE1  | 2:47:B:LEU:HA   | 39       | 0.11          |
| (1,233) | 2:46:B:TYR:HE2  | 2:47:B:LEU:HA   | 39       | 0.11          |
| (1,225) | 2:45:B:LEU:HG   | 2:54:B:PHE:HE1  | 6        | 0.11          |
| (1,225) | 2:45:B:LEU:HG   | 2:54:B:PHE:HE2  | 6        | 0.11          |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD1  | 20       | 0.11          |
| (1,210) | 1:16:A:LEU:HD21 | 1:19:A:TYR:HD2  | 20       | 0.11          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD1  | 20       | 0.11          |
| (1,210) | 1:16:A:LEU:HD22 | 1:19:A:TYR:HD2  | 20       | 0.11          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD1  | 20       | 0.11          |
| (1,210) | 1:16:A:LEU:HD23 | 1:19:A:TYR:HD2  | 20       | 0.11          |
| (1,191) | 2:54:B:PHE:HA   | 2:55:B:PHE:H    | 17       | 0.11          |
| (1,178) | 2:50:B:GLY:H    | 2:51:B:GLU:H    | 24       | 0.11          |
| (1,150) | 2:44:B:ALA:H    | 2:47:B:LEU:HD11 | 22       | 0.11          |
| (1,150) | 2:44:B:ALA:H    | 2:47:B:LEU:HD12 | 22       | 0.11          |
| (1,150) | 2:44:B:ALA:H    | 2:47:B:LEU:HD13 | 22       | 0.11          |
| (1,150) | 2:44:B:ALA:H    | 2:47:B:LEU:HD21 | 22       | 0.11          |
| (1,150) | 2:44:B:ALA:H    | 2:47:B:LEU:HD22 | 22       | 0.11          |
| (1,150) | 2:44:B:ALA:H    | 2:47:B:LEU:HD23 | 22       | 0.11          |
| (1,142) | 2:42:B:VAL:HB   | 2:43:B:GLU:H    | 10       | 0.11          |
| (1,127) | 2:37:B:CYS:H    | 2:40:B:HIS:HB3  | 16       | 0.11          |
| (1,105) | 1:21:A:ASN:H    | 1:21:A:ASN:HB2  | 17       | 0.11          |
| (1,84)  | 2:54:B:PHE:HB2  | 2:55:B:PHE:H    | 5        | 0.11          |
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE1  | 6        | 0.11          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,44)  | 1:16:A:LEU:H    | 1:19:A:TYR:HE2 | 6        | 0.11          |
| (1,25)  | 2:36:B:LEU:HD11 | 2:45:B:LEU:H   | 27       | 0.11          |
| (1,25)  | 2:36:B:LEU:HD12 | 2:45:B:LEU:H   | 27       | 0.11          |
| (1,25)  | 2:36:B:LEU:HD13 | 2:45:B:LEU:H   | 27       | 0.11          |
| (1,25)  | 2:36:B:LEU:HD21 | 2:45:B:LEU:H   | 27       | 0.11          |
| (1,25)  | 2:36:B:LEU:HD22 | 2:45:B:LEU:H   | 27       | 0.11          |
| (1,25)  | 2:36:B:LEU:HD23 | 2:45:B:LEU:H   | 27       | 0.11          |
| (1,17)  | 2:48:B:VAL:HG21 | 2:49:B:CYS:H   | 12       | 0.11          |
| (1,17)  | 2:48:B:VAL:HG22 | 2:49:B:CYS:H   | 12       | 0.11          |
| (1,17)  | 2:48:B:VAL:HG23 | 2:49:B:CYS:H   | 12       | 0.11          |
| (1,5)   | 1:10:A:ILE:HD11 | 2:35:B:HIS:HE1 | 36       | 0.11          |
| (1,5)   | 1:10:A:ILE:HD12 | 2:35:B:HIS:HE1 | 36       | 0.11          |
| (1,5)   | 1:10:A:ILE:HD13 | 2:35:B:HIS:HE1 | 36       | 0.11          |
| (3,32)  | 1:1:A:GLY:O     | 1:5:A:GLN:N    | 32       | 0.1           |
| (3,27)  | 1:3:A:VAL:O     | 1:7:A:CYS:H    | 4        | 0.1           |
| (3,25)  | 1:12:A:SER:O    | 1:16:A:LEU:H   | 39       | 0.1           |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H   | 4        | 0.1           |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H   | 9        | 0.1           |
| (3,21)  | 1:15:A:GLN:O    | 1:18:A:ASN:H   | 27       | 0.1           |
| (3,19)  | 1:16:A:LEU:O    | 1:19:A:TYR:H   | 22       | 0.1           |
| (3,17)  | 1:17:A:GLU:O    | 1:20:A:CYS:H   | 36       | 0.1           |
| (3,11)  | 2:41:B:LEU:O    | 2:45:B:LEU:H   | 35       | 0.1           |
| (3,8)   | 2:43:B:GLU:O    | 2:47:B:LEU:N   | 35       | 0.1           |
| (3,7)   | 2:43:B:GLU:O    | 2:47:B:LEU:H   | 6        | 0.1           |
| (3,7)   | 2:43:B:GLU:O    | 2:47:B:LEU:H   | 40       | 0.1           |
| (3,5)   | 2:44:B:ALA:O    | 2:48:B:VAL:H   | 11       | 0.1           |
| (3,3)   | 2:45:B:LEU:O    | 2:49:B:CYS:H   | 30       | 0.1           |
| (3,1)   | 2:46:B:TYR:O    | 2:50:B:GLY:H   | 16       | 0.1           |
| (1,452) | 1:16:A:LEU:HD11 | 2:45:B:LEU:HG  | 13       | 0.1           |
| (1,452) | 1:16:A:LEU:HD12 | 2:45:B:LEU:HG  | 13       | 0.1           |
| (1,452) | 1:16:A:LEU:HD13 | 2:45:B:LEU:HG  | 13       | 0.1           |
| (1,452) | 1:16:A:LEU:HD21 | 2:45:B:LEU:HG  | 13       | 0.1           |
| (1,452) | 1:16:A:LEU:HD22 | 2:45:B:LEU:HG  | 13       | 0.1           |
| (1,452) | 1:16:A:LEU:HD23 | 2:45:B:LEU:HG  | 13       | 0.1           |
| (1,450) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB1 | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB2 | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB3 | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB1 | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB2 | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB3 | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB1 | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB2 | 34       | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,450) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB3  | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD21 | 2:44:B:ALA:HB1  | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD21 | 2:44:B:ALA:HB2  | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD21 | 2:44:B:ALA:HB3  | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD22 | 2:44:B:ALA:HB1  | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD22 | 2:44:B:ALA:HB2  | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD22 | 2:44:B:ALA:HB3  | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD23 | 2:44:B:ALA:HB1  | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD23 | 2:44:B:ALA:HB2  | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD23 | 2:44:B:ALA:HB3  | 34       | 0.1           |
| (1,450) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB1  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB2  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD11 | 2:44:B:ALA:HB3  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB1  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB2  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD12 | 2:44:B:ALA:HB3  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB1  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB2  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD13 | 2:44:B:ALA:HB3  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD21 | 2:44:B:ALA:HB1  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD21 | 2:44:B:ALA:HB2  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD21 | 2:44:B:ALA:HB3  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD22 | 2:44:B:ALA:HB1  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD22 | 2:44:B:ALA:HB2  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD22 | 2:44:B:ALA:HB3  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD23 | 2:44:B:ALA:HB1  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD23 | 2:44:B:ALA:HB2  | 36       | 0.1           |
| (1,450) | 1:16:A:LEU:HD23 | 2:44:B:ALA:HB3  | 36       | 0.1           |
| (1,416) | 1:12:A:SER:HB2  | 1:14:A:TYR:HD1  | 2        | 0.1           |
| (1,416) | 1:12:A:SER:HB2  | 1:14:A:TYR:HD2  | 2        | 0.1           |
| (1,416) | 1:12:A:SER:HB3  | 1:14:A:TYR:HD1  | 2        | 0.1           |
| (1,416) | 1:12:A:SER:HB3  | 1:14:A:TYR:HD2  | 2        | 0.1           |
| (1,375) | 2:45:B:LEU:HA   | 2:48:B:VAL:HB   | 24       | 0.1           |
| (1,327) | 2:43:B:GLU:H    | 2:45:B:LEU:HB2  | 26       | 0.1           |
| (1,327) | 2:43:B:GLU:H    | 2:45:B:LEU:HB2  | 28       | 0.1           |
| (1,296) | 2:46:B:TYR:HB2  | 2:47:B:LEU:HD11 | 31       | 0.1           |
| (1,296) | 2:46:B:TYR:HB2  | 2:47:B:LEU:HD12 | 31       | 0.1           |
| (1,296) | 2:46:B:TYR:HB2  | 2:47:B:LEU:HD13 | 31       | 0.1           |
| (1,296) | 2:46:B:TYR:HB2  | 2:47:B:LEU:HD21 | 31       | 0.1           |
| (1,296) | 2:46:B:TYR:HB2  | 2:47:B:LEU:HD22 | 31       | 0.1           |
| (1,296) | 2:46:B:TYR:HB2  | 2:47:B:LEU:HD23 | 31       | 0.1           |
| (1,296) | 2:46:B:TYR:HB3  | 2:47:B:LEU:HD11 | 31       | 0.1           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,296) | 2:46:B:TYR:HB3 | 2:47:B:LEU:HD12 | 31       | 0.1           |
| (1,296) | 2:46:B:TYR:HB3 | 2:47:B:LEU:HD13 | 31       | 0.1           |
| (1,296) | 2:46:B:TYR:HB3 | 2:47:B:LEU:HD21 | 31       | 0.1           |
| (1,296) | 2:46:B:TYR:HB3 | 2:47:B:LEU:HD22 | 31       | 0.1           |
| (1,296) | 2:46:B:TYR:HB3 | 2:47:B:LEU:HD23 | 31       | 0.1           |
| (1,215) | 2:56:B:TYR:H   | 2:57:B:THR:H    | 11       | 0.1           |
| (1,178) | 2:50:B:GLY:H   | 2:51:B:GLU:H    | 39       | 0.1           |
| (1,142) | 2:42:B:VAL:HB  | 2:43:B:GLU:H    | 20       | 0.1           |
| (1,127) | 2:37:B:CYS:H   | 2:40:B:HIS:HB3  | 24       | 0.1           |
| (1,127) | 2:37:B:CYS:H   | 2:40:B:HIS:HB3  | 32       | 0.1           |
| (1,117) | 2:32:B:VAL:HB  | 2:33:B:ASN:H    | 34       | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found