



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 09:03 PM UTC

PDB ID : 5U4K / pdb\_00005u4k  
Title : NMR structure of the complex between the KIX domain of CBP and the transactivation domain 1 of p65  
Authors : Lecoq, L.; Raiola, L.; Chabot, P.R.; Cyr, N.; Arseneault, G.; Omichinski, J.G.  
Deposited on : 2016-12-05

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                                                             |

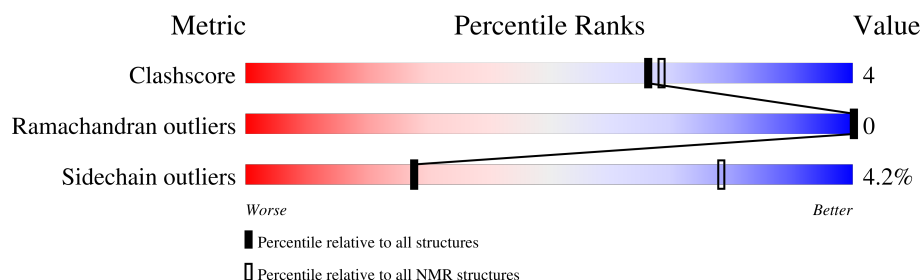
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 89%.

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     | 87     |                  |
| 2   | B     | 33     |                  |

## 2 Ensemble composition and analysis

This entry contains 20 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: *lowest energy*.

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

| Well-defined (core) protein residues |                                  |                   |              |
|--------------------------------------|----------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)            | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:590-A:665, B:536-B:551<br>(92) | 0.78              | 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 4 clusters. No single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1922 atoms, of which 956 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CREB-binding protein.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 87       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1469  | 459 | 740 | 136 | 132 | 2 |       |

- Molecule 2 is a protein called Transcription factor p65.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 2   | B     | 33       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 453   | 146 | 216 | 35 | 55 | 1 |       |

There are 3 discrepancies between the modelled and reference sequences:

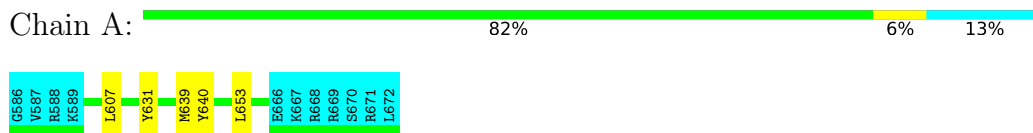
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | 519     | GLY      | -      | expression tag      | UNP Q04206 |
| B     | 520     | SER      | -      | expression tag      | UNP Q04206 |
| B     | 523     | TYR      | LEU    | engineered mutation | UNP Q04206 |

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

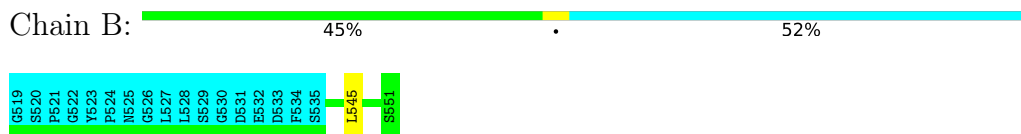
### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: CREB-binding protein



- Molecule 2: Transcription factor p65

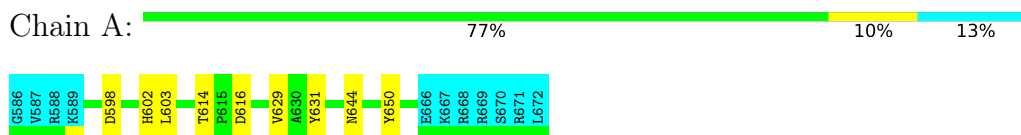


### 4.2 Scores per residue for each member of the ensemble

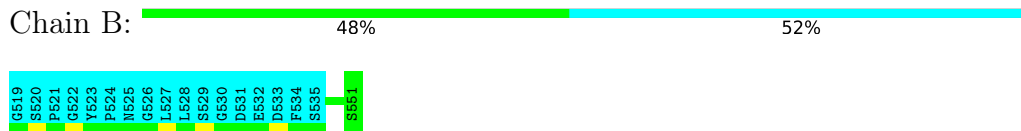
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: CREB-binding protein

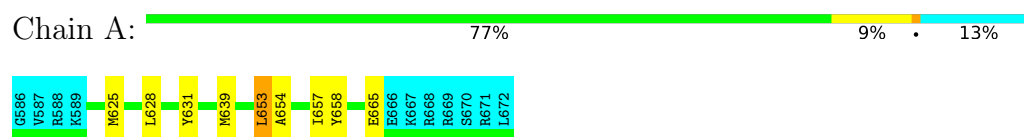


- Molecule 2: Transcription factor p65

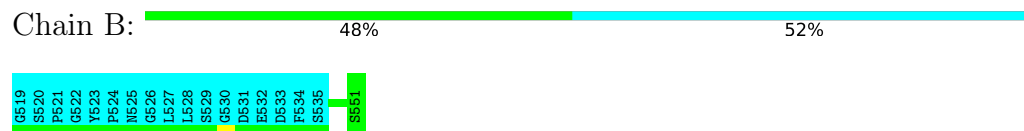


### 4.2.2 Score per residue for model 2

- Molecule 1: CREB-binding protein

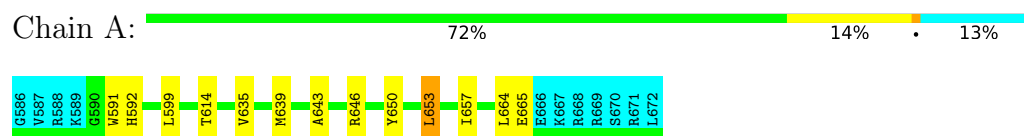


- Molecule 2: Transcription factor p65

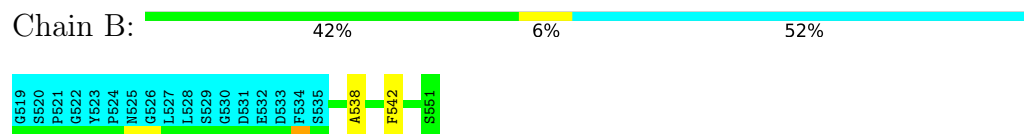


### 4.2.3 Score per residue for model 3

- Molecule 1: CREB-binding protein

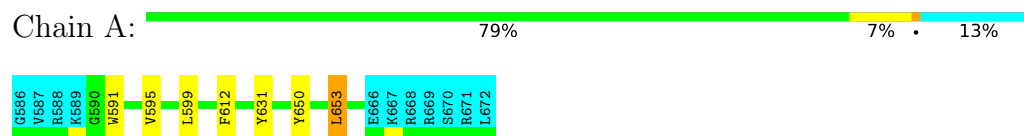


- Molecule 2: Transcription factor p65

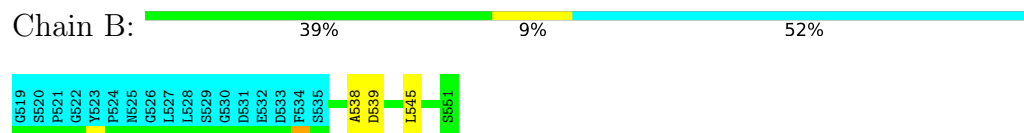


### 4.2.4 Score per residue for model 4

- Molecule 1: CREB-binding protein



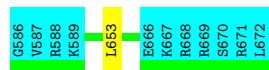
- Molecule 2: Transcription factor p65



### 4.2.5 Score per residue for model 5

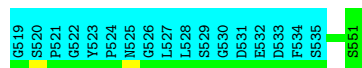
- Molecule 1: CREB-binding protein

Chain A:  86% 13%



- Molecule 2: Transcription factor p65

Chain B:  48% 52%



### 4.2.6 Score per residue for model 6

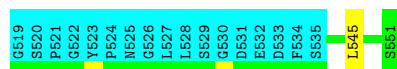
- Molecule 1: CREB-binding protein

Chain A:  76% 10% 13%



- Molecule 2: Transcription factor p65

Chain B:  45% 52%



### 4.2.7 Score per residue for model 7

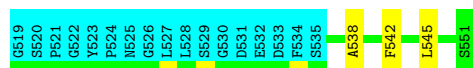
- Molecule 1: CREB-binding protein

Chain A:  76% 10% 13%



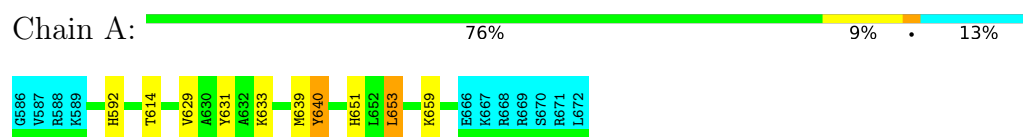
- Molecule 2: Transcription factor p65

Chain B:  39% 9% 52%



### 4.2.8 Score per residue for model 8

- Molecule 1: CREB-binding protein

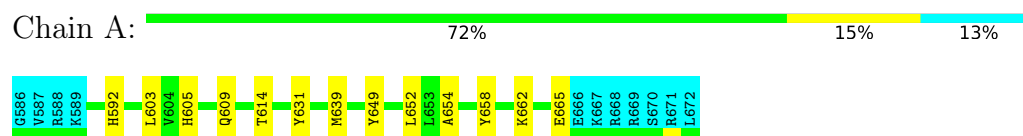


- Molecule 2: Transcription factor p65

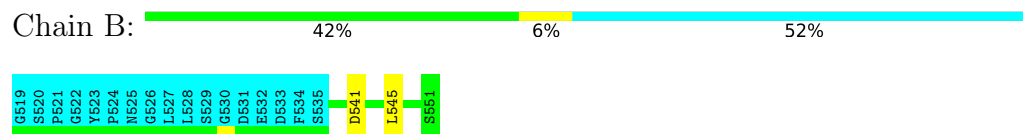


### 4.2.9 Score per residue for model 9

- Molecule 1: CREB-binding protein

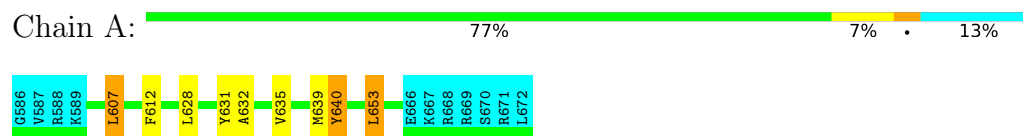


- Molecule 2: Transcription factor p65

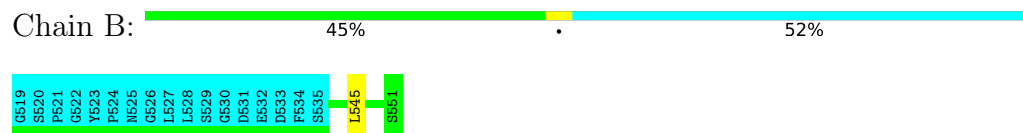


### 4.2.10 Score per residue for model 10

- Molecule 1: CREB-binding protein

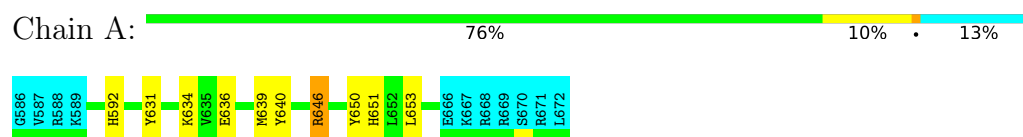


- Molecule 2: Transcription factor p65

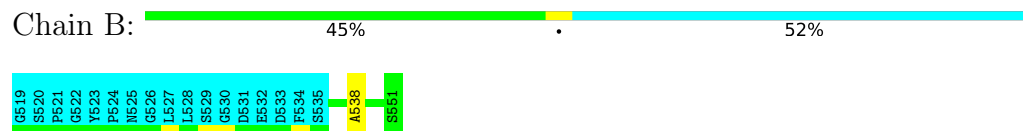


### 4.2.11 Score per residue for model 11

- Molecule 1: CREB-binding protein

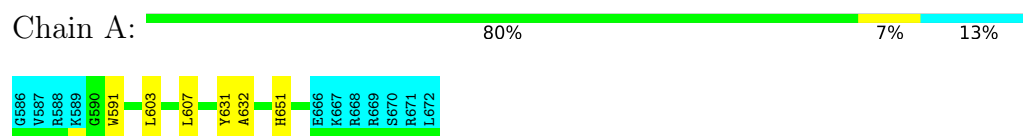


- Molecule 2: Transcription factor p65

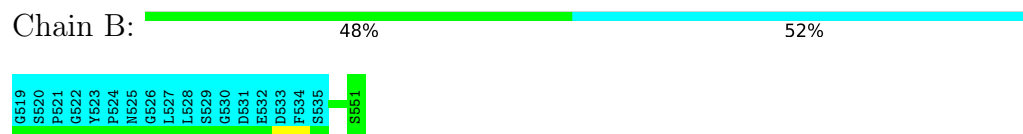


### 4.2.12 Score per residue for model 12

- Molecule 1: CREB-binding protein

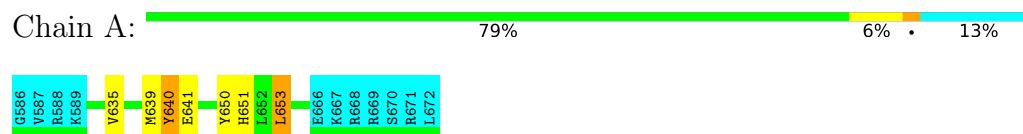


- Molecule 2: Transcription factor p65

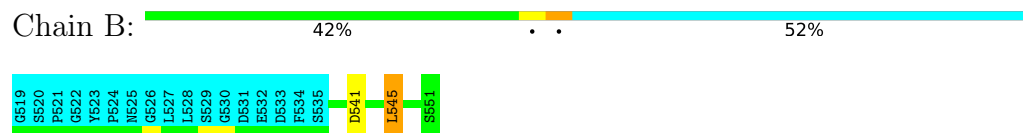


### 4.2.13 Score per residue for model 13

- Molecule 1: CREB-binding protein

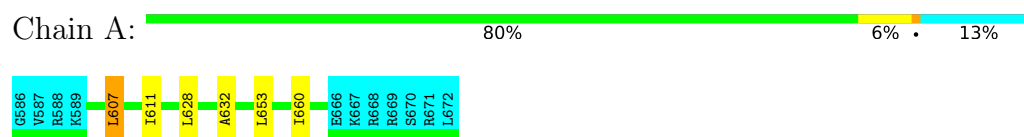


- Molecule 2: Transcription factor p65

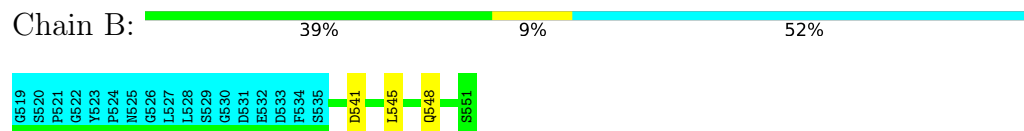


#### 4.2.14 Score per residue for model 14

- Molecule 1: CREB-binding protein

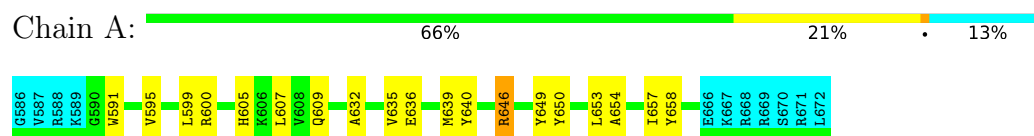


- Molecule 2: Transcription factor p65

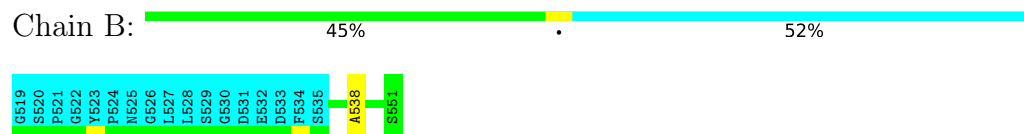


#### 4.2.15 Score per residue for model 15

- Molecule 1: CREB-binding protein

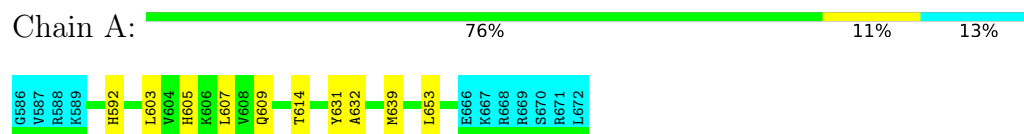


- Molecule 2: Transcription factor p65

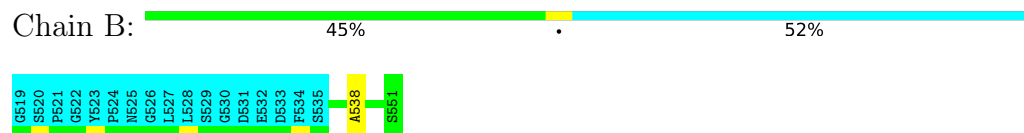


#### 4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: CREB-binding protein

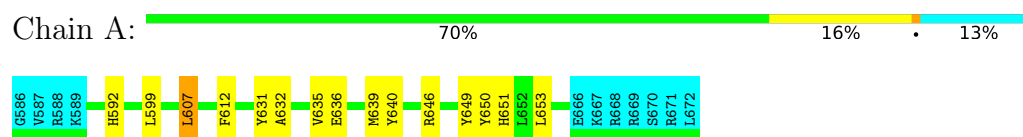


- Molecule 2: Transcription factor p65

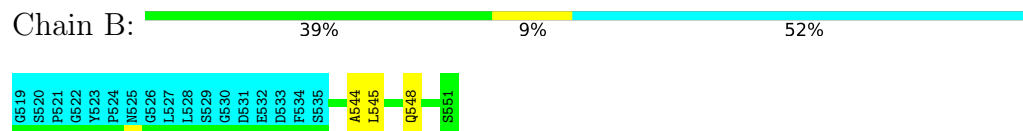


### 4.2.17 Score per residue for model 17

- Molecule 1: CREB-binding protein

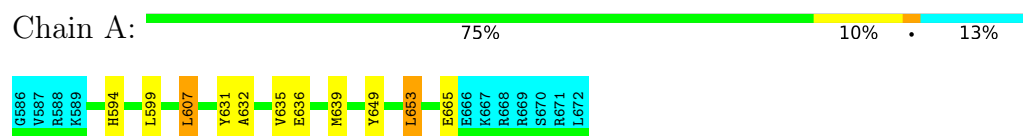


- Molecule 2: Transcription factor p65

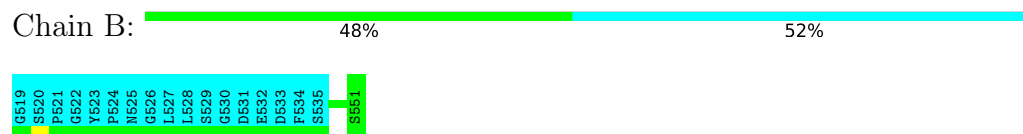


### 4.2.18 Score per residue for model 18

- Molecule 1: CREB-binding protein

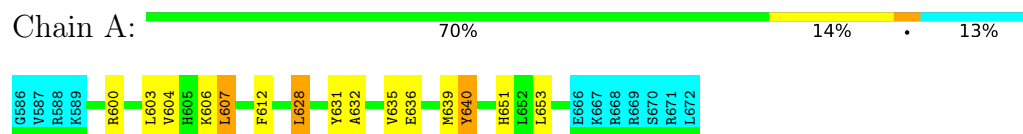


- Molecule 2: Transcription factor p65

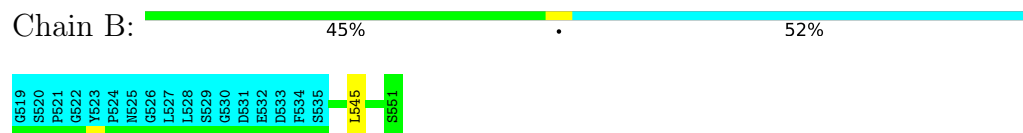


### 4.2.19 Score per residue for model 19

- Molecule 1: CREB-binding protein



- Molecule 2: Transcription factor p65



#### 4.2.20 Score per residue for model 20

- Molecule 1: CREB-binding protein

Chain A:  77% 8% 13%



- Molecule 2: Transcription factor p65

Chain B:  36% 12% 52%



## 5 Refinement protocol and experimental data overview

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

Of the 260 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| ARIA          | structure calculation |         |
| CNS           | 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                       | 1439           |
| Number of shifts mapped to atoms             | 1439           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 89%            |

## 6 Model quality [i](#)

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

There are no covalent bond-length or bond-angle outliers.

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 0.3±0.5   |
| All | All   | 0         | 7         |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 631 | TYR  | Sidechain | 7              |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 632   | 626      | 621      | 5±3     |
| 2   | B     | 117   | 113      | 113      | 1±1     |
| All | All   | 14980 | 14780    | 13946    | 114     |

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 4.

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

| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:607:LEU:HD13 | 1:A:632:ALA:HB1 | 0.94     | 1.34        | 19     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:636:GLU:HA   | 1:A:639:MET:HE2  | 0.77     | 1.56        | 11     | 3     |
| 1:A:639:MET:SD   | 1:A:653:LEU:HB2  | 0.69     | 2.26        | 3      | 10    |
| 1:A:607:LEU:HD13 | 1:A:632:ALA:CB   | 0.65     | 2.17        | 19     | 2     |
| 1:A:612:PHE:CG   | 2:B:545:LEU:HD13 | 0.63     | 2.28        | 19     | 1     |
| 1:A:640:TYR:C    | 1:A:640:TYR:CD1  | 0.61     | 2.78        | 8      | 3     |
| 1:A:612:PHE:CD2  | 2:B:545:LEU:HD13 | 0.61     | 2.30        | 19     | 3     |
| 1:A:640:TYR:C    | 1:A:640:TYR:CD2  | 0.61     | 2.78        | 19     | 1     |
| 1:A:646:ARG:O    | 1:A:650:TYR:CD1  | 0.58     | 2.56        | 15     | 4     |
| 1:A:650:TYR:HA   | 1:A:653:LEU:HD23 | 0.57     | 1.76        | 4      | 2     |
| 1:A:607:LEU:HD23 | 1:A:632:ALA:HB1  | 0.57     | 1.75        | 17     | 4     |
| 1:A:639:MET:SD   | 1:A:653:LEU:HG   | 0.57     | 2.40        | 10     | 1     |
| 1:A:639:MET:SD   | 1:A:652:LEU:HB3  | 0.55     | 2.41        | 6      | 2     |
| 1:A:591:TRP:NE1  | 1:A:595:VAL:HG21 | 0.55     | 2.17        | 15     | 1     |
| 1:A:625:MET:N    | 2:B:545:LEU:HD21 | 0.55     | 2.16        | 20     | 1     |
| 1:A:612:PHE:CG   | 2:B:545:LEU:CD1  | 0.54     | 2.90        | 19     | 1     |
| 1:A:635:VAL:O    | 1:A:639:MET:HG2  | 0.54     | 2.02        | 6      | 1     |
| 1:A:599:LEU:HD21 | 1:A:650:TYR:OH   | 0.54     | 2.03        | 6      | 2     |
| 1:A:635:VAL:O    | 1:A:639:MET:HG3  | 0.54     | 2.03        | 19     | 5     |
| 1:A:640:TYR:CE2  | 1:A:641:GLU:HG3  | 0.53     | 2.38        | 13     | 1     |
| 1:A:603:LEU:CD1  | 1:A:649:TYR:OH   | 0.52     | 2.58        | 9      | 1     |
| 1:A:628:LEU:HD23 | 1:A:631:TYR:CD2  | 0.51     | 2.40        | 2      | 2     |
| 1:A:592:HIS:C    | 1:A:592:HIS:CD2  | 0.51     | 2.88        | 7      | 1     |
| 1:A:603:LEU:O    | 1:A:653:LEU:HD21 | 0.51     | 2.06        | 16     | 1     |
| 1:A:607:LEU:HD22 | 1:A:653:LEU:CD1  | 0.50     | 2.37        | 16     | 1     |
| 1:A:605:HIS:O    | 1:A:609:GLN:HG2  | 0.49     | 2.07        | 15     | 4     |
| 1:A:619:ALA:HB1  | 2:B:545:LEU:HD11 | 0.49     | 1.85        | 7      | 1     |
| 1:A:619:ALA:O    | 2:B:545:LEU:CD1  | 0.49     | 2.61        | 7      | 1     |
| 2:B:541:ASP:O    | 2:B:545:LEU:HG   | 0.48     | 2.08        | 14     | 2     |
| 1:A:636:GLU:OE2  | 1:A:649:TYR:OH   | 0.48     | 2.31        | 15     | 1     |
| 1:A:612:PHE:O    | 1:A:612:PHE:CD1  | 0.48     | 2.67        | 7      | 1     |
| 1:A:611:ILE:HG12 | 1:A:660:ILE:HG21 | 0.47     | 1.87        | 14     | 1     |
| 1:A:654:ALA:O    | 1:A:658:TYR:CD1  | 0.47     | 2.68        | 15     | 3     |
| 1:A:639:MET:SD   | 1:A:649:TYR:O    | 0.47     | 2.73        | 17     | 1     |
| 1:A:619:ALA:O    | 2:B:545:LEU:HD11 | 0.46     | 2.10        | 7      | 1     |
| 1:A:607:LEU:HB2  | 1:A:653:LEU:HD11 | 0.46     | 1.85        | 16     | 1     |
| 1:A:605:HIS:HA   | 1:A:608:VAL:HG22 | 0.46     | 1.87        | 7      | 1     |
| 1:A:640:TYR:CD1  | 1:A:640:TYR:C    | 0.46     | 2.93        | 20     | 1     |
| 1:A:607:LEU:CD1  | 1:A:632:ALA:HB1  | 0.46     | 2.25        | 19     | 1     |
| 1:A:614:THR:CG2  | 1:A:616:ASP:O    | 0.46     | 2.64        | 1      | 1     |
| 2:B:538:ALA:O    | 2:B:542:PHE:HB2  | 0.46     | 2.11        | 20     | 1     |
| 1:A:604:VAL:HG23 | 1:A:636:GLU:OE1  | 0.45     | 2.12        | 19     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:607:LEU:CD2  | 1:A:632:ALA:HB1  | 0.45     | 2.41        | 15     | 2     |
| 1:A:639:MET:HE3  | 1:A:649:TYR:CE1  | 0.45     | 2.46        | 18     | 1     |
| 1:A:639:MET:SD   | 1:A:653:LEU:HB3  | 0.45     | 2.51        | 13     | 1     |
| 1:A:628:LEU:O    | 1:A:631:TYR:HB2  | 0.45     | 2.11        | 10     | 1     |
| 1:A:639:MET:SD   | 1:A:652:LEU:CB   | 0.44     | 3.04        | 6      | 1     |
| 1:A:607:LEU:HD22 | 1:A:653:LEU:HD11 | 0.44     | 1.87        | 16     | 1     |
| 1:A:598:ASP:O    | 1:A:602:HIS:CD2  | 0.44     | 2.70        | 1      | 1     |
| 1:A:640:TYR:CD2  | 1:A:641:GLU:HG3  | 0.44     | 2.48        | 13     | 1     |
| 1:A:595:VAL:HG13 | 1:A:599:LEU:HD23 | 0.44     | 1.90        | 4      | 1     |
| 1:A:612:PHE:CZ   | 2:B:545:LEU:HB3  | 0.44     | 2.48        | 4      | 2     |
| 1:A:649:TYR:C    | 1:A:649:TYR:CD1  | 0.44     | 2.94        | 9      | 1     |
| 1:A:640:TYR:CE2  | 1:A:641:GLU:CG   | 0.43     | 3.02        | 13     | 1     |
| 1:A:640:TYR:CD1  | 1:A:640:TYR:O    | 0.43     | 2.71        | 8      | 1     |
| 1:A:611:ILE:HG21 | 1:A:628:LEU:HD21 | 0.42     | 1.91        | 7      | 1     |
| 1:A:600:ARG:HG2  | 1:A:636:GLU:OE2  | 0.42     | 2.14        | 15     | 1     |
| 1:A:603:LEU:HA   | 1:A:606:LYS:HB2  | 0.42     | 1.90        | 19     | 1     |
| 2:B:544:ALA:O    | 2:B:548:GLN:HG2  | 0.42     | 2.15        | 17     | 1     |
| 1:A:632:ALA:O    | 1:A:635:VAL:HG22 | 0.42     | 2.14        | 19     | 1     |
| 1:A:591:TRP:CD1  | 1:A:592:HIS:N    | 0.42     | 2.88        | 3      | 1     |
| 1:A:595:VAL:HG22 | 1:A:599:LEU:HD23 | 0.42     | 1.92        | 15     | 1     |
| 1:A:607:LEU:HD11 | 1:A:635:VAL:CG2  | 0.42     | 2.45        | 19     | 1     |
| 2:B:542:PHE:O    | 2:B:542:PHE:CD1  | 0.41     | 2.73        | 7      | 1     |
| 2:B:542:PHE:CD1  | 2:B:542:PHE:C    | 0.41     | 2.98        | 3      | 1     |
| 2:B:545:LEU:HD23 | 2:B:548:GLN:NE2  | 0.41     | 2.31        | 14     | 1     |
| 1:A:646:ARG:HG3  | 1:A:650:TYR:CE1  | 0.41     | 2.51        | 3      | 1     |
| 1:A:603:LEU:HD21 | 1:A:650:TYR:CE2  | 0.40     | 2.50        | 1      | 1     |
| 1:A:600:ARG:O    | 1:A:636:GLU:OE1  | 0.40     | 2.40        | 19     | 1     |
| 1:A:591:TRP:CH2  | 1:A:643:ALA:O    | 0.40     | 2.74        | 3      | 1     |
| 1:A:629:VAL:O    | 1:A:633:LYS:HG3  | 0.40     | 2.16        | 8      | 1     |
| 2:B:541:ASP:O    | 2:B:545:LEU:HB2  | 0.40     | 2.16        | 13     | 1     |
| 1:A:662:LYS:O    | 1:A:665:GLU:HB2  | 0.40     | 2.16        | 9      | 1     |
| 1:A:592:HIS:CD2  | 1:A:592:HIS:O    | 0.40     | 2.74        | 7      | 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     | 76/87 (87%)     | 76±0 (100±1%) | 0±0 (0±1%) | 0±0 (0±0%) | 100         | 100 |
| 2   | B     | 15/33 (45%)     | 15±0 (100±0%) | 0±0 (0±0%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 1820/2400 (76%) | 1815 (100%)   | 5 (0%)     | 0 (0%)     | 100         | 100 |

There are no Ramachandran outliers.

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|-------------|----|
| 1   | A     | 67/77 (87%)     | 64±1 (95±2%) | 3±1 (5±2%) | 24          | 74 |
| 2   | B     | 14/27 (52%)     | 14±0 (99±2%) | 0±0 (1±2%) | 73          | 96 |
| All | All   | 1620/2080 (78%) | 1552 (96%)   | 68 (4%)    | 28          | 78 |

All 22 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 653 | LEU  | 12             |
| 1   | A     | 640 | TYR  | 9              |
| 1   | A     | 592 | HIS  | 6              |
| 1   | A     | 651 | HIS  | 6              |
| 1   | A     | 607 | LEU  | 5              |
| 1   | A     | 614 | THR  | 4              |
| 1   | A     | 657 | ILE  | 3              |
| 1   | A     | 665 | GLU  | 3              |
| 1   | A     | 628 | LEU  | 3              |
| 1   | A     | 625 | MET  | 2              |
| 1   | A     | 646 | ARG  | 2              |
| 1   | A     | 635 | VAL  | 2              |
| 1   | A     | 599 | LEU  | 2              |
| 1   | A     | 629 | VAL  | 1              |
| 1   | A     | 664 | LEU  | 1              |
| 1   | A     | 641 | GLU  | 1              |
| 1   | A     | 634 | LYS  | 1              |
| 1   | A     | 603 | LEU  | 1              |
| 2   | B     | 545 | LEU  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 594 | HIS  | 1              |
| 1   | A     | 626 | GLU  | 1              |
| 2   | B     | 541 | ASP  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 87% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *referenced\_CSfile.str*

#### 7.1.1 Bookkeeping [i](#)

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                  | 1439 |
| Number of shifts mapped to atoms        | 1439 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 1    |

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 119      | $-0.11 \pm 0.15$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 112      | $0.36 \pm 0.07$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 110      | $0.12 \pm 0.18$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 110      | $0.22 \pm 0.18$                 | None needed ( $< 0.5$ ppm) |

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1151 atoms were assigned a chemical shift out of a possible 1287. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 452/456 (99%) | 183/183 (100%) | 180/184 (98%)   | 89/89 (100%)    |
| Sidechain | 625/714 (88%) | 416/464 (90%)  | 203/225 (90%)   | 6/25 (24%)      |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 74/117 (63%)    | 37/56 (66%)          | 36/50 (72%)           | 1/11 (9%)             |
| Overall  | 1151/1287 (89%) | 636/703 (90%)        | 419/459 (91%)         | 96/125 (77%)          |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1439 atoms were assigned a chemical shift out of a possible 1659. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 573/597 (96%)   | 234/242 (97%)        | 229/240 (95%)         | 110/115 (96%)         |
| Sidechain | 776/926 (84%)   | 515/598 (86%)        | 254/288 (88%)         | 7/40 (18%)            |
| Aromatic  | 90/136 (66%)    | 45/65 (69%)          | 44/60 (73%)           | 1/11 (9%)             |
| Overall   | 1439/1659 (87%) | 794/905 (88%)        | 527/588 (90%)         | 118/166 (71%)         |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

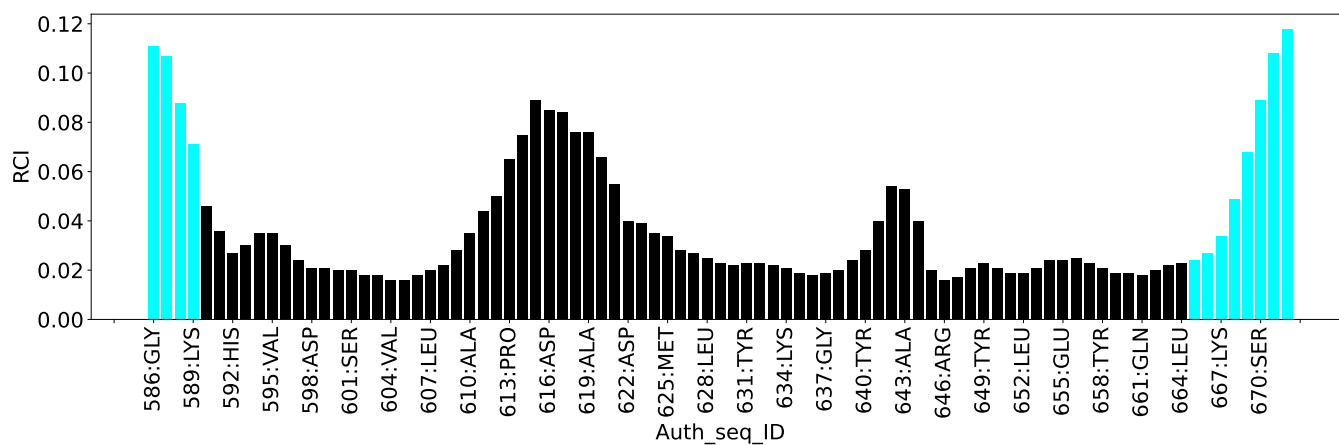
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 589 | LYS  | HB3  | 0.28       | 0.46 – 3.04         | -5.7    |

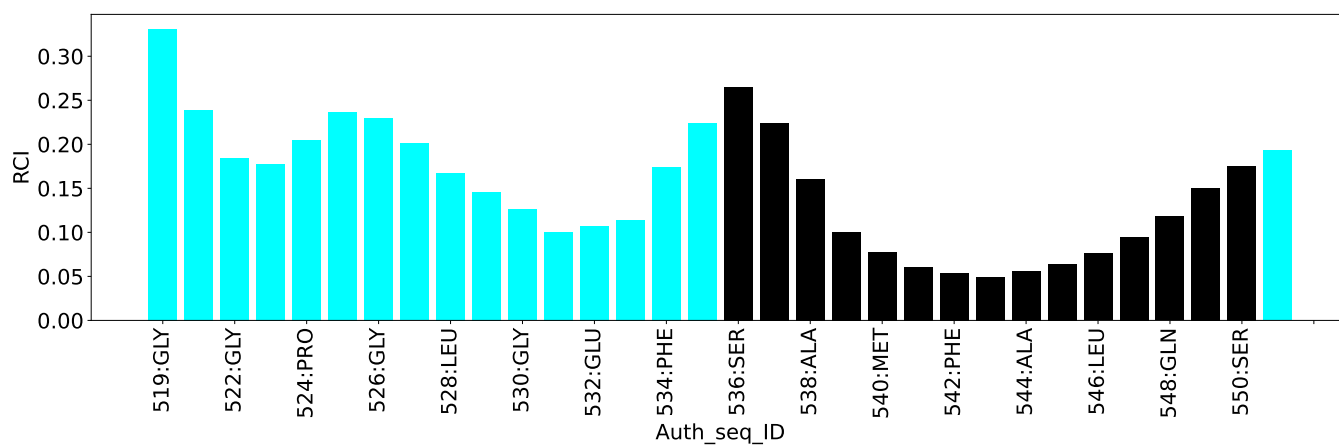
#### 7.1.5 Random Coil Index (RCI) plots ⓘ

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 [i](#)

### 8.1 Conformationally restricting restraints [i](#)

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                                | 1327  |
| Intra-residue ( $ i-j =0$ )                              | 853   |
| Sequential ( $ i-j =1$ )                                 | 172   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 164   |
| Long range ( $ i-j \geq 5$ )                             | 104   |
| Inter-chain                                              | 34    |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 201   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 12.7  |
| Number of long range restraints per residue <sup>1</sup> | 0.9   |

<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 [i](#)

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 [i](#)

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)  | 52.0                                   | 0.2     |
| 0.2-0.5 (Medium) | 98.7                                   | 0.5     |
| >0.5 (Large)     | 210.4                                  | 9.68    |

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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 14.7                                   | 3.68    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

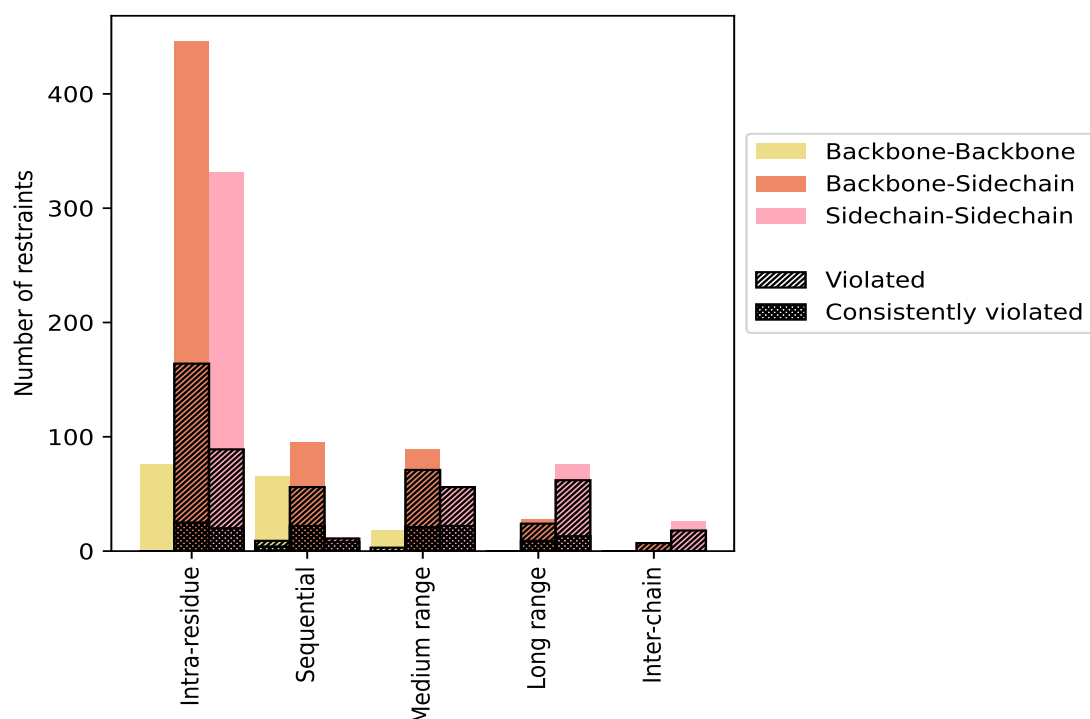
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>853</b>  | <b>64.3</b>    | <b>253</b>            | <b>29.7</b>    | <b>19.1</b>    | <b>45</b>                          | <b>5.3</b>     | <b>3.4</b>     |
| Backbone-Backbone                                                           | 76          | 5.7            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 446         | 33.6           | 164                   | 36.8           | 12.4           | 25                                 | 5.6            | 1.9            |
| Sidechain-Sidechain                                                         | 331         | 24.9           | 89                    | 26.9           | 6.7            | 20                                 | 6.0            | 1.5            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>172</b>  | <b>13.0</b>    | <b>76</b>             | <b>44.2</b>    | <b>5.7</b>     | <b>34</b>                          | <b>19.8</b>    | <b>2.6</b>     |
| Backbone-Backbone                                                           | 65          | 4.9            | 9                     | 13.8           | 0.7            | 4                                  | 6.2            | 0.3            |
| Backbone-Sidechain                                                          | 95          | 7.2            | 56                    | 58.9           | 4.2            | 22                                 | 23.2           | 1.7            |
| Sidechain-Sidechain                                                         | 12          | 0.9            | 11                    | 91.7           | 0.8            | 8                                  | 66.7           | 0.6            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>164</b>  | <b>12.4</b>    | <b>130</b>            | <b>79.3</b>    | <b>9.8</b>     | <b>43</b>                          | <b>26.2</b>    | <b>3.2</b>     |
| Backbone-Backbone                                                           | 18          | 1.4            | 3                     | 16.7           | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 89          | 6.7            | 71                    | 79.8           | 5.4            | 21                                 | 23.6           | 1.6            |
| Sidechain-Sidechain                                                         | 57          | 4.3            | 56                    | 98.2           | 4.2            | 22                                 | 38.6           | 1.7            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>104</b>  | <b>7.8</b>     | <b>86</b>             | <b>82.7</b>    | <b>6.5</b>     | <b>22</b>                          | <b>21.2</b>    | <b>1.7</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 28          | 2.1            | 24                    | 85.7           | 1.8            | 9                                  | 32.1           | 0.7            |
| Sidechain-Sidechain                                                         | 76          | 5.7            | 62                    | 81.6           | 4.7            | 13                                 | 17.1           | 1.0            |
| <b>Inter-chain</b>                                                          | <b>34</b>   | <b>2.6</b>     | <b>25</b>             | <b>73.5</b>    | <b>1.9</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 8           | 0.6            | 7                     | 87.5           | 0.5            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 26          | 2.0            | 18                    | 69.2           | 1.4            | 0                                  | 0.0            | 0.0            |
| Hydrogen bond                                                               | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Disulfide bond                                                              | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Total</b>                                                                | <b>1327</b> | <b>100.0</b>   | <b>570</b>            | <b>43.0</b>    | <b>43.0</b>    | <b>144</b>                         | <b>10.9</b>    | <b>10.9</b>    |
| Backbone-Backbone                                                           | 159         | 12.0           | 12                    | 7.5            | 0.9            | 4                                  | 2.5            | 0.3            |
| Backbone-Sidechain                                                          | 666         | 50.2           | 322                   | 48.3           | 24.3           | 77                                 | 11.6           | 5.8            |
| Sidechain-Sidechain                                                         | 502         | 37.8           | 236                   | 47.0           | 17.8           | 63                                 | 12.5           | 4.7            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 149                  | 57              | 92              | 63              | 12              | 373   | 1.14     | 7.31    | 1.27                | 0.64       |
| 2        | 138                  | 62              | 97              | 61              | 13              | 371   | 1.22     | 9.68    | 1.43                | 0.66       |
| 3        | 146                  | 63              | 90              | 58              | 5               | 362   | 1.08     | 8.28    | 1.18                | 0.66       |
| 4        | 142                  | 60              | 89              | 64              | 8               | 363   | 1.11     | 7.47    | 1.22                | 0.64       |
| 5        | 134                  | 54              | 83              | 64              | 11              | 346   | 1.1      | 7.47    | 1.13                | 0.66       |
| 6        | 144                  | 59              | 94              | 58              | 11              | 366   | 1.14     | 7.57    | 1.24                | 0.63       |
| 7        | 146                  | 59              | 92              | 61              | 13              | 371   | 1.1      | 6.84    | 1.16                | 0.68       |
| 8        | 144                  | 62              | 87              | 62              | 9               | 364   | 1.22     | 7.41    | 1.36                | 0.64       |
| 9        | 141                  | 57              | 88              | 58              | 11              | 355   | 1.05     | 6.38    | 1.08                | 0.58       |
| 10       | 136                  | 57              | 89              | 54              | 14              | 350   | 1.09     | 7.01    | 1.23                | 0.6        |

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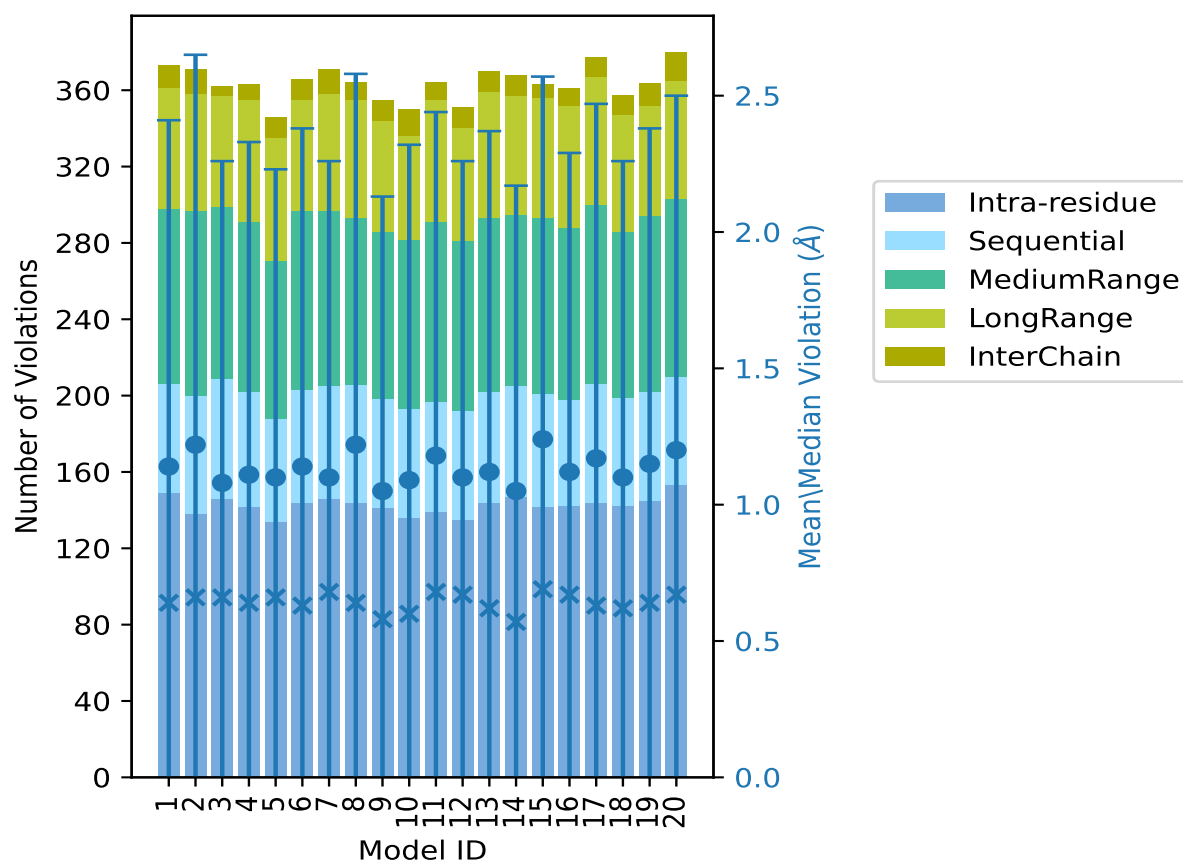
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 139                  | 58              | 94              | 64              | 9               | 364   | 1.18     | 7.05    | 1.26                | 0.68       |
| 12       | 135                  | 57              | 89              | 59              | 11              | 351   | 1.1      | 8.21    | 1.16                | 0.67       |
| 13       | 144                  | 58              | 91              | 66              | 11              | 370   | 1.12     | 7.44    | 1.25                | 0.62       |
| 14       | 147                  | 58              | 90              | 62              | 11              | 368   | 1.05     | 7.43    | 1.12                | 0.57       |
| 15       | 142                  | 59              | 92              | 63              | 7               | 363   | 1.24     | 7.46    | 1.33                | 0.69       |
| 16       | 142                  | 56              | 90              | 64              | 9               | 361   | 1.12     | 7.34    | 1.17                | 0.67       |
| 17       | 144                  | 62              | 94              | 67              | 10              | 377   | 1.17     | 7.41    | 1.3                 | 0.63       |
| 18       | 142                  | 57              | 87              | 61              | 10              | 357   | 1.1      | 7.62    | 1.16                | 0.62       |
| 19       | 145                  | 57              | 92              | 58              | 12              | 364   | 1.15     | 6.62    | 1.23                | 0.64       |
| 20       | 153                  | 57              | 93              | 62              | 15              | 380   | 1.2      | 7.32    | 1.3                 | 0.67       |

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

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

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



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

### 9.3 Distance violation statistics for the ensemble

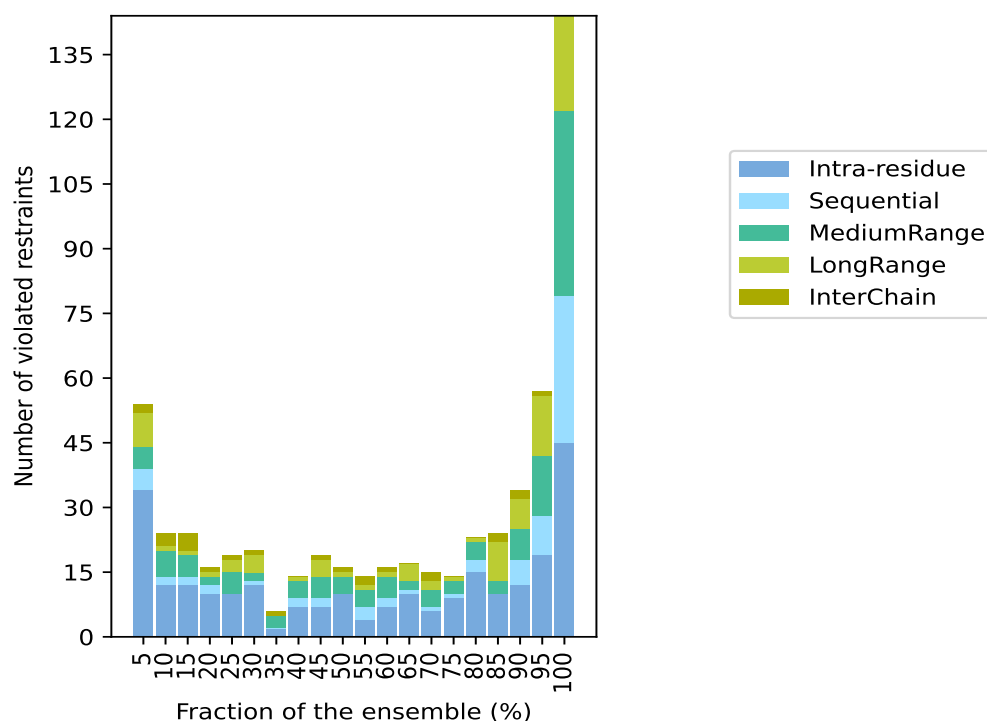
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 757(IR:600, SQ:96, MR:34, LR:18, IC:9) restraints are not 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>       | %     |
| 34                            | 5               | 5               | 8               | 2               | 54    | 1                        | 5.0   |
| 12                            | 2               | 6               | 1               | 3               | 24    | 2                        | 10.0  |
| 12                            | 2               | 5               | 1               | 4               | 24    | 3                        | 15.0  |
| 10                            | 2               | 2               | 1               | 1               | 16    | 4                        | 20.0  |
| 10                            | 0               | 5               | 3               | 1               | 19    | 5                        | 25.0  |
| 12                            | 1               | 2               | 4               | 1               | 20    | 6                        | 30.0  |
| 2                             | 0               | 3               | 0               | 1               | 6     | 7                        | 35.0  |
| 7                             | 2               | 4               | 1               | 0               | 14    | 8                        | 40.0  |
| 7                             | 2               | 5               | 4               | 1               | 19    | 9                        | 45.0  |
| 10                            | 0               | 4               | 1               | 1               | 16    | 10                       | 50.0  |
| 4                             | 3               | 4               | 1               | 2               | 14    | 11                       | 55.0  |
| 7                             | 2               | 5               | 1               | 1               | 16    | 12                       | 60.0  |
| 10                            | 1               | 2               | 4               | 0               | 17    | 13                       | 65.0  |
| 6                             | 1               | 4               | 2               | 2               | 15    | 14                       | 70.0  |
| 9                             | 1               | 3               | 1               | 0               | 14    | 15                       | 75.0  |
| 15                            | 3               | 4               | 1               | 0               | 23    | 16                       | 80.0  |
| 10                            | 0               | 3               | 9               | 2               | 24    | 17                       | 85.0  |
| 12                            | 6               | 7               | 7               | 2               | 34    | 18                       | 90.0  |
| 19                            | 9               | 14              | 14              | 1               | 57    | 19                       | 95.0  |
| 45                            | 34              | 43              | 22              | 0               | 144   | 20                       | 100.0 |

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

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

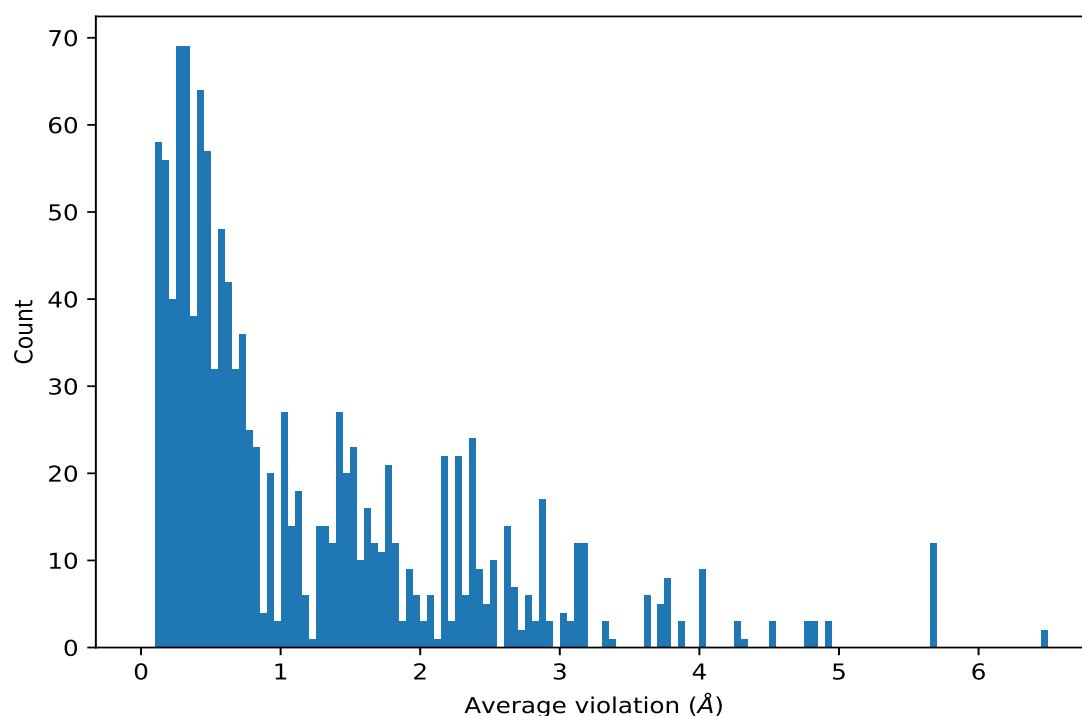
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,7)   | 1:628:A:LEU:HD22 | 1:625:A:MET:HE2 | 20                  | 5.67     | 1.8                 | 6.2        |
| (1,7)   | 1:628:A:LEU:HD22 | 1:625:A:MET:HE1 | 20                  | 5.67     | 1.8                 | 6.2        |
| (1,7)   | 1:628:A:LEU:HD23 | 1:625:A:MET:HE2 | 20                  | 5.67     | 1.8                 | 6.2        |
| (1,7)   | 1:628:A:LEU:HD22 | 1:625:A:MET:HE3 | 20                  | 5.67     | 1.8                 | 6.2        |
| (1,7)   | 1:628:A:LEU:HD21 | 1:625:A:MET:HE3 | 20                  | 5.67     | 1.8                 | 6.2        |
| (1,7)   | 1:628:A:LEU:HD21 | 1:625:A:MET:HE2 | 20                  | 5.67     | 1.8                 | 6.2        |
| (1,7)   | 1:628:A:LEU:HD23 | 1:625:A:MET:HE1 | 20                  | 5.67     | 1.8                 | 6.2        |
| (1,7)   | 1:628:A:LEU:HD23 | 1:625:A:MET:HE3 | 20                  | 5.67     | 1.8                 | 6.2        |
| (1,7)   | 1:628:A:LEU:HD21 | 1:625:A:MET:HE1 | 20                  | 5.67     | 1.8                 | 6.2        |
| (1,482) | 1:664:A:LEU:HD13 | 1:667:A:LYS:HD2 | 20                  | 5.66     | 1.46                | 5.46       |
| (1,482) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HD2 | 20                  | 5.66     | 1.46                | 5.46       |
| (1,482) | 1:664:A:LEU:HD12 | 1:667:A:LYS:HD2 | 20                  | 5.66     | 1.46                | 5.46       |
| (1,433) | 1:656:A:LYS:HG2  | 1:639:A:MET:HE1 | 20                  | 4.82     | 1.78                | 5.63       |
| (1,433) | 1:656:A:LYS:HG2  | 1:639:A:MET:HE2 | 20                  | 4.82     | 1.78                | 5.63       |
| (1,433) | 1:656:A:LYS:HG2  | 1:639:A:MET:HE3 | 20                  | 4.82     | 1.78                | 5.63       |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3 | 20                  | 4.33     | 1.19                | 4.76       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,487) | 1:664:A:LEU:HD13 | 1:667:A:LYS:HG2  | 20                  | 4.26     | 0.75                | 4.32       |
| (1,487) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HG2  | 20                  | 4.26     | 0.75                | 4.32       |
| (1,487) | 1:664:A:LEU:HD12 | 1:667:A:LYS:HG2  | 20                  | 4.26     | 0.75                | 4.32       |
| (1,625) | 1:632:A:ALA:HB1  | 1:628:A:LEU:HD12 | 20                  | 4.04     | 0.83                | 4.28       |
| (1,625) | 1:632:A:ALA:HB1  | 1:628:A:LEU:HD11 | 20                  | 4.04     | 0.83                | 4.28       |
| (1,625) | 1:632:A:ALA:HB2  | 1:628:A:LEU:HD12 | 20                  | 4.04     | 0.83                | 4.28       |
| (1,625) | 1:632:A:ALA:HB1  | 1:628:A:LEU:HD13 | 20                  | 4.04     | 0.83                | 4.28       |
| (1,625) | 1:632:A:ALA:HB2  | 1:628:A:LEU:HD13 | 20                  | 4.04     | 0.83                | 4.28       |
| (1,625) | 1:632:A:ALA:HB3  | 1:628:A:LEU:HD12 | 20                  | 4.04     | 0.83                | 4.28       |
| (1,625) | 1:632:A:ALA:HB3  | 1:628:A:LEU:HD11 | 20                  | 4.04     | 0.83                | 4.28       |
| (1,625) | 1:632:A:ALA:HB2  | 1:628:A:LEU:HD11 | 20                  | 4.04     | 0.83                | 4.28       |
| (1,625) | 1:632:A:ALA:HB3  | 1:628:A:LEU:HD13 | 20                  | 4.04     | 0.83                | 4.28       |
| (1,438) | 1:672:A:LEU:HD11 | 1:671:A:ARG:HG3  | 20                  | 3.85     | 0.59                | 3.92       |
| (1,438) | 1:672:A:LEU:HD13 | 1:671:A:ARG:HG3  | 20                  | 3.85     | 0.59                | 3.92       |
| (1,438) | 1:672:A:LEU:HD12 | 1:671:A:ARG:HG3  | 20                  | 3.85     | 0.59                | 3.92       |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 20                  | 3.72     | 0.71                | 3.74       |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD22 | 20                  | 3.71     | 1.09                | 3.98       |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD23 | 20                  | 3.71     | 1.09                | 3.98       |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD21 | 20                  | 3.71     | 1.09                | 3.98       |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 20                  | 3.7      | 0.38                | 3.84       |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 20                  | 3.37     | 0.71                | 3.36       |
| (1,626) | 1:625:A:MET:HE2  | 1:628:A:LEU:HD13 | 20                  | 3.19     | 0.77                | 3.1        |
| (1,626) | 1:625:A:MET:HE1  | 1:628:A:LEU:HD12 | 20                  | 3.19     | 0.77                | 3.1        |
| (1,626) | 1:625:A:MET:HE2  | 1:628:A:LEU:HD11 | 20                  | 3.19     | 0.77                | 3.1        |
| (1,626) | 1:625:A:MET:HE3  | 1:628:A:LEU:HD13 | 20                  | 3.19     | 0.77                | 3.1        |
| (1,626) | 1:625:A:MET:HE2  | 1:628:A:LEU:HD12 | 20                  | 3.19     | 0.77                | 3.1        |
| (1,626) | 1:625:A:MET:HE1  | 1:628:A:LEU:HD11 | 20                  | 3.19     | 0.77                | 3.1        |
| (1,626) | 1:625:A:MET:HE3  | 1:628:A:LEU:HD12 | 20                  | 3.19     | 0.77                | 3.1        |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE1  | 20                  | 3.1      | 2.12                | 2.38       |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE2  | 20                  | 3.1      | 2.12                | 2.38       |
| (1,148) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE1  | 20                  | 3.1      | 2.12                | 2.38       |
| (1,148) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE2  | 20                  | 3.1      | 2.12                | 2.38       |
| (1,148) | 1:635:A:VAL:HG11 | 1:631:A:TYR:HE1  | 20                  | 3.1      | 2.12                | 2.38       |
| (1,148) | 1:635:A:VAL:HG11 | 1:631:A:TYR:HE2  | 20                  | 3.1      | 2.12                | 2.38       |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD23 | 20                  | 3.07     | 1.18                | 3.42       |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD22 | 20                  | 3.07     | 1.18                | 3.42       |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD21 | 20                  | 3.07     | 1.18                | 3.42       |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD23 | 20                  | 3.03     | 1.51                | 3.36       |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD21 | 20                  | 3.03     | 1.51                | 3.36       |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD22 | 20                  | 3.03     | 1.51                | 3.36       |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 20                  | 3.0      | 0.13                | 2.96       |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 20                  | 2.89     | 0.65                | 3.08       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD11 | 20                  | 2.88     | 1.19                | 2.89       |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD11 | 20                  | 2.88     | 1.19                | 2.89       |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD13 | 20                  | 2.88     | 1.19                | 2.89       |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD13 | 20                  | 2.88     | 1.19                | 2.89       |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD12 | 20                  | 2.88     | 1.19                | 2.89       |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD12 | 20                  | 2.88     | 1.19                | 2.89       |
| (1,961) | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 20                  | 2.88     | 0.43                | 2.86       |
| (1,547) | 1:603:A:LEU:HD13 | 1:606:A:LYS:HD2  | 20                  | 2.87     | 0.67                | 3.0        |
| (1,547) | 1:603:A:LEU:HD11 | 1:606:A:LYS:HD2  | 20                  | 2.87     | 0.67                | 3.0        |
| (1,547) | 1:603:A:LEU:HD12 | 1:606:A:LYS:HD2  | 20                  | 2.87     | 0.67                | 3.0        |
| (1,430) | 1:664:A:LEU:HD22 | 1:661:A:GLN:HA   | 20                  | 2.85     | 0.26                | 2.87       |
| (1,430) | 1:664:A:LEU:HD23 | 1:661:A:GLN:HA   | 20                  | 2.85     | 0.26                | 2.87       |
| (1,430) | 1:664:A:LEU:HD21 | 1:661:A:GLN:HA   | 20                  | 2.85     | 0.26                | 2.87       |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD13 | 20                  | 2.85     | 0.29                | 2.84       |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD11 | 20                  | 2.85     | 0.29                | 2.84       |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD12 | 20                  | 2.85     | 0.29                | 2.84       |
| (1,477) | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG21 | 20                  | 2.83     | 0.36                | 2.62       |
| (1,477) | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG22 | 20                  | 2.83     | 0.36                | 2.62       |
| (1,477) | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG23 | 20                  | 2.83     | 0.36                | 2.62       |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD21 | 20                  | 2.78     | 0.85                | 3.08       |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD23 | 20                  | 2.78     | 0.85                | 3.08       |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD22 | 20                  | 2.78     | 0.85                | 3.08       |
| (1,927) | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 20                  | 2.69     | 0.42                | 2.81       |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 20                  | 2.64     | 0.72                | 2.86       |
| (1,20)  | 1:660:A:ILE:HG22 | 1:664:A:LEU:HD22 | 20                  | 2.62     | 0.25                | 2.64       |
| (1,20)  | 1:660:A:ILE:HG22 | 1:664:A:LEU:HD21 | 20                  | 2.62     | 0.25                | 2.64       |
| (1,20)  | 1:660:A:ILE:HG23 | 1:664:A:LEU:HD22 | 20                  | 2.62     | 0.25                | 2.64       |
| (1,20)  | 1:660:A:ILE:HG21 | 1:664:A:LEU:HD22 | 20                  | 2.62     | 0.25                | 2.64       |
| (1,20)  | 1:660:A:ILE:HG21 | 1:664:A:LEU:HD23 | 20                  | 2.62     | 0.25                | 2.64       |
| (1,20)  | 1:660:A:ILE:HG21 | 1:664:A:LEU:HD21 | 20                  | 2.62     | 0.25                | 2.64       |
| (1,20)  | 1:660:A:ILE:HG22 | 1:664:A:LEU:HD23 | 20                  | 2.62     | 0.25                | 2.64       |
| (1,679) | 1:643:A:ALA:H    | 1:652:A:LEU:HD23 | 20                  | 2.61     | 0.32                | 2.7        |
| (1,679) | 1:643:A:ALA:H    | 1:652:A:LEU:HD21 | 20                  | 2.61     | 0.32                | 2.7        |
| (1,679) | 1:643:A:ALA:H    | 1:652:A:LEU:HD22 | 20                  | 2.61     | 0.32                | 2.7        |
| (1,129) | 1:652:A:LEU:HD23 | 1:649:A:TYR:HA   | 20                  | 2.6      | 0.2                 | 2.54       |
| (1,129) | 1:652:A:LEU:HD21 | 1:649:A:TYR:HA   | 20                  | 2.6      | 0.2                 | 2.54       |
| (1,129) | 1:652:A:LEU:HD22 | 1:649:A:TYR:HA   | 20                  | 2.6      | 0.2                 | 2.54       |
| (1,33)  | 1:652:A:LEU:HD23 | 1:643:A:ALA:HB1  | 20                  | 2.42     | 0.19                | 2.46       |
| (1,33)  | 1:652:A:LEU:HD21 | 1:643:A:ALA:HB1  | 20                  | 2.42     | 0.19                | 2.46       |
| (1,33)  | 1:652:A:LEU:HD23 | 1:643:A:ALA:HB3  | 20                  | 2.42     | 0.19                | 2.46       |
| (1,33)  | 1:652:A:LEU:HD22 | 1:643:A:ALA:HB3  | 20                  | 2.42     | 0.19                | 2.46       |
| (1,33)  | 1:652:A:LEU:HD22 | 1:643:A:ALA:HB2  | 20                  | 2.42     | 0.19                | 2.46       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,33)  | 1:652:A:LEU:HD21 | 1:643:A:ALA:HB2  | 20                  | 2.42     | 0.19                | 2.46       |
| (1,33)  | 1:652:A:LEU:HD21 | 1:643:A:ALA:HB3  | 20                  | 2.42     | 0.19                | 2.46       |
| (1,33)  | 1:652:A:LEU:HD23 | 1:643:A:ALA:HB2  | 20                  | 2.42     | 0.19                | 2.46       |
| (1,33)  | 1:652:A:LEU:HD22 | 1:643:A:ALA:HB1  | 20                  | 2.42     | 0.19                | 2.46       |
| (1,4)   | 1:629:A:VAL:HG22 | 1:625:A:MET:HE3  | 20                  | 2.36     | 0.76                | 2.04       |
| (1,4)   | 1:629:A:VAL:HG21 | 1:625:A:MET:HE2  | 20                  | 2.36     | 0.76                | 2.04       |
| (1,4)   | 1:629:A:VAL:HG21 | 1:625:A:MET:HE3  | 20                  | 2.36     | 0.76                | 2.04       |
| (1,4)   | 1:629:A:VAL:HG21 | 1:625:A:MET:HE1  | 20                  | 2.36     | 0.76                | 2.04       |
| (1,4)   | 1:629:A:VAL:HG23 | 1:625:A:MET:HE1  | 20                  | 2.36     | 0.76                | 2.04       |
| (1,4)   | 1:629:A:VAL:HG22 | 1:625:A:MET:HE2  | 20                  | 2.36     | 0.76                | 2.04       |
| (1,4)   | 1:629:A:VAL:HG23 | 1:625:A:MET:HE3  | 20                  | 2.36     | 0.76                | 2.04       |
| (1,4)   | 1:629:A:VAL:HG22 | 1:625:A:MET:HE1  | 20                  | 2.36     | 0.76                | 2.04       |
| (1,4)   | 1:629:A:VAL:HG23 | 1:625:A:MET:HE2  | 20                  | 2.36     | 0.76                | 2.04       |
| (1,5)   | 1:608:A:VAL:HG21 | 1:625:A:MET:HE3  | 20                  | 2.27     | 1.04                | 2.01       |
| (1,5)   | 1:608:A:VAL:HG21 | 1:625:A:MET:HE2  | 20                  | 2.27     | 1.04                | 2.01       |
| (1,5)   | 1:608:A:VAL:HG23 | 1:625:A:MET:HE1  | 20                  | 2.27     | 1.04                | 2.01       |
| (1,5)   | 1:608:A:VAL:HG23 | 1:625:A:MET:HE2  | 20                  | 2.27     | 1.04                | 2.01       |
| (1,5)   | 1:608:A:VAL:HG23 | 1:625:A:MET:HE3  | 20                  | 2.27     | 1.04                | 2.01       |
| (1,5)   | 1:608:A:VAL:HG22 | 1:625:A:MET:HE2  | 20                  | 2.27     | 1.04                | 2.01       |
| (1,5)   | 1:608:A:VAL:HG22 | 1:625:A:MET:HE3  | 20                  | 2.27     | 1.04                | 2.01       |
| (1,5)   | 1:608:A:VAL:HG22 | 1:625:A:MET:HE1  | 20                  | 2.27     | 1.04                | 2.01       |
| (1,376) | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 20                  | 2.25     | 0.55                | 2.18       |
| (1,376) | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG11 | 20                  | 2.25     | 0.55                | 2.18       |
| (1,376) | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG13 | 20                  | 2.25     | 0.55                | 2.18       |
| (1,467) | 1:652:A:LEU:HD23 | 1:643:A:ALA:HA   | 20                  | 2.24     | 0.16                | 2.25       |
| (1,467) | 1:652:A:LEU:HD21 | 1:643:A:ALA:HA   | 20                  | 2.24     | 0.16                | 2.25       |
| (1,467) | 1:652:A:LEU:HD22 | 1:643:A:ALA:HA   | 20                  | 2.24     | 0.16                | 2.25       |
| (1,596) | 1:632:A:ALA:HB1  | 1:635:A:VAL:HG21 | 20                  | 2.19     | 0.77                | 2.5        |
| (1,596) | 1:632:A:ALA:HB2  | 1:635:A:VAL:HG22 | 20                  | 2.19     | 0.77                | 2.5        |
| (1,596) | 1:632:A:ALA:HB1  | 1:635:A:VAL:HG23 | 20                  | 2.19     | 0.77                | 2.5        |
| (1,596) | 1:632:A:ALA:HB3  | 1:635:A:VAL:HG22 | 20                  | 2.19     | 0.77                | 2.5        |
| (1,596) | 1:632:A:ALA:HB2  | 1:635:A:VAL:HG21 | 20                  | 2.19     | 0.77                | 2.5        |
| (1,596) | 1:632:A:ALA:HB3  | 1:635:A:VAL:HG23 | 20                  | 2.19     | 0.77                | 2.5        |
| (1,596) | 1:632:A:ALA:HB1  | 1:635:A:VAL:HG22 | 20                  | 2.19     | 0.77                | 2.5        |
| (1,596) | 1:632:A:ALA:HB2  | 1:635:A:VAL:HG23 | 20                  | 2.19     | 0.77                | 2.5        |
| (1,596) | 1:632:A:ALA:HB3  | 1:635:A:VAL:HG21 | 20                  | 2.19     | 0.77                | 2.5        |
| (1,559) | 1:603:A:LEU:HD21 | 1:600:A:ARG:HA   | 20                  | 2.17     | 0.37                | 2.06       |
| (1,559) | 1:603:A:LEU:HD22 | 1:600:A:ARG:HA   | 20                  | 2.17     | 0.37                | 2.06       |
| (1,559) | 1:603:A:LEU:HD23 | 1:600:A:ARG:HA   | 20                  | 2.17     | 0.37                | 2.06       |
| (1,499) | 1:639:A:MET:HG3  | 1:652:A:LEU:HD22 | 20                  | 2.16     | 0.36                | 2.17       |
| (1,499) | 1:639:A:MET:HG3  | 1:652:A:LEU:HD23 | 20                  | 2.16     | 0.36                | 2.17       |
| (1,499) | 1:639:A:MET:HG3  | 1:652:A:LEU:HD21 | 20                  | 2.16     | 0.36                | 2.17       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,738) | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 20                  | 2.1      | 0.38                | 2.0        |
| (1,294) | 1:604:A:VAL:HG11 | 1:633:A:LYS:HD2  | 20                  | 2.04     | 0.46                | 1.86       |
| (1,294) | 1:604:A:VAL:HG12 | 1:633:A:LYS:HD2  | 20                  | 2.04     | 0.46                | 1.86       |
| (1,294) | 1:604:A:VAL:HG13 | 1:633:A:LYS:HD2  | 20                  | 2.04     | 0.46                | 1.86       |
| (1,318) | 1:652:A:LEU:HA   | 1:652:A:LEU:HD13 | 20                  | 1.93     | 0.06                | 1.94       |
| (1,318) | 1:652:A:LEU:HA   | 1:652:A:LEU:HD12 | 20                  | 1.93     | 0.06                | 1.94       |
| (1,318) | 1:652:A:LEU:HA   | 1:652:A:LEU:HD11 | 20                  | 1.93     | 0.06                | 1.94       |
| (1,303) | 1:664:A:LEU:HD13 | 1:664:A:LEU:HA   | 20                  | 1.92     | 0.16                | 1.97       |
| (1,303) | 1:664:A:LEU:HD11 | 1:664:A:LEU:HA   | 20                  | 1.92     | 0.16                | 1.97       |
| (1,303) | 1:664:A:LEU:HD12 | 1:664:A:LEU:HA   | 20                  | 1.92     | 0.16                | 1.97       |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD12 | 20                  | 1.8      | 0.33                | 1.76       |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD13 | 20                  | 1.8      | 0.33                | 1.76       |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD11 | 20                  | 1.8      | 0.33                | 1.76       |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 20                  | 1.79     | 0.43                | 1.59       |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD22 | 20                  | 1.75     | 0.22                | 1.76       |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD23 | 20                  | 1.75     | 0.22                | 1.76       |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD21 | 20                  | 1.75     | 0.22                | 1.76       |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG21 | 20                  | 1.73     | 0.35                | 1.8        |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG23 | 20                  | 1.73     | 0.35                | 1.8        |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG22 | 20                  | 1.73     | 0.35                | 1.8        |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 20                  | 1.69     | 0.15                | 1.7        |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB2  | 20                  | 1.68     | 0.25                | 1.77       |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB1  | 20                  | 1.68     | 0.25                | 1.77       |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB3  | 20                  | 1.68     | 0.25                | 1.77       |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB3  | 20                  | 1.68     | 0.14                | 1.68       |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB2  | 20                  | 1.68     | 0.14                | 1.68       |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB1  | 20                  | 1.68     | 0.14                | 1.68       |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 20                  | 1.67     | 0.52                | 1.52       |
| (1,87)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 20                  | 1.53     | 0.55                | 1.33       |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD11 | 20                  | 1.53     | 0.12                | 1.52       |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD12 | 20                  | 1.53     | 0.12                | 1.52       |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD13 | 20                  | 1.53     | 0.12                | 1.52       |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD11 | 20                  | 1.49     | 0.17                | 1.54       |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD12 | 20                  | 1.49     | 0.17                | 1.54       |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD13 | 20                  | 1.49     | 0.17                | 1.54       |
| (1,423) | 1:629:A:VAL:HG13 | 1:626:A:GLU:HG2  | 20                  | 1.48     | 0.54                | 1.61       |
| (1,423) | 1:629:A:VAL:HG11 | 1:626:A:GLU:HG2  | 20                  | 1.48     | 0.54                | 1.61       |
| (1,423) | 1:629:A:VAL:HG12 | 1:626:A:GLU:HG2  | 20                  | 1.48     | 0.54                | 1.61       |
| (1,278) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 20                  | 1.48     | 0.51                | 1.87       |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD12 | 20                  | 1.48     | 0.31                | 1.58       |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD13 | 20                  | 1.48     | 0.31                | 1.58       |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD11 | 20                  | 1.48     | 0.31                | 1.58       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB1  | 20                  | 1.43     | 0.13                | 1.44       |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB3  | 20                  | 1.43     | 0.13                | 1.44       |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB2  | 20                  | 1.43     | 0.13                | 1.44       |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 20                  | 1.41     | 0.05                | 1.42       |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD11 | 20                  | 1.39     | 0.39                | 1.35       |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD13 | 20                  | 1.39     | 0.39                | 1.35       |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD12 | 20                  | 1.39     | 0.39                | 1.35       |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 20                  | 1.37     | 0.04                | 1.37       |
| (1,610) | 1:599:A:LEU:HD21 | 1:603:A:LEU:HD22 | 20                  | 1.34     | 0.76                | 1.04       |
| (1,610) | 1:599:A:LEU:HD22 | 1:603:A:LEU:HD23 | 20                  | 1.34     | 0.76                | 1.04       |
| (1,610) | 1:599:A:LEU:HD22 | 1:603:A:LEU:HD21 | 20                  | 1.34     | 0.76                | 1.04       |
| (1,610) | 1:599:A:LEU:HD23 | 1:603:A:LEU:HD22 | 20                  | 1.34     | 0.76                | 1.04       |
| (1,610) | 1:599:A:LEU:HD21 | 1:603:A:LEU:HD21 | 20                  | 1.34     | 0.76                | 1.04       |
| (1,610) | 1:599:A:LEU:HD23 | 1:603:A:LEU:HD21 | 20                  | 1.34     | 0.76                | 1.04       |
| (1,610) | 1:599:A:LEU:HD22 | 1:603:A:LEU:HD22 | 20                  | 1.34     | 0.76                | 1.04       |
| (1,610) | 1:599:A:LEU:HD23 | 1:603:A:LEU:HD23 | 20                  | 1.34     | 0.76                | 1.04       |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 20                  | 1.34     | 0.23                | 1.23       |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 20                  | 1.31     | 0.08                | 1.33       |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 20                  | 1.28     | 0.36                | 1.22       |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 20                  | 1.16     | 0.32                | 1.13       |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 20                  | 1.15     | 0.75                | 0.82       |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD23 | 20                  | 1.11     | 0.23                | 1.04       |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD21 | 20                  | 1.11     | 0.23                | 1.04       |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD22 | 20                  | 1.11     | 0.23                | 1.04       |
| (1,286) | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 20                  | 1.1      | 0.14                | 1.12       |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD21 | 20                  | 1.09     | 0.07                | 1.1        |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD22 | 20                  | 1.09     | 0.07                | 1.1        |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD23 | 20                  | 1.09     | 0.07                | 1.1        |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 20                  | 1.06     | 0.2                 | 1.03       |
| (1,581) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 20                  | 1.06     | 0.27                | 1.12       |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 20                  | 1.06     | 0.31                | 0.91       |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 20                  | 1.04     | 0.39                | 1.18       |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 20                  | 1.04     | 0.74                | 0.62       |
| (1,639) | 1:652:A:LEU:HD23 | 1:642:A:SER:HB2  | 20                  | 1.03     | 0.34                | 1.01       |
| (1,639) | 1:652:A:LEU:HD21 | 1:642:A:SER:HB2  | 20                  | 1.03     | 0.34                | 1.01       |
| (1,639) | 1:652:A:LEU:HD22 | 1:642:A:SER:HB2  | 20                  | 1.03     | 0.34                | 1.01       |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 20                  | 1.03     | 0.3                 | 1.04       |
| (1,812) | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 20                  | 1.02     | 0.24                | 0.92       |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 20                  | 1.0      | 0.11                | 1.0        |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 20                  | 1.0      | 0.11                | 1.0        |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 20                  | 0.96     | 0.29                | 0.91       |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 20                  | 0.92     | 0.22                | 0.98       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD21 | 20                  | 0.89     | 0.08                | 0.92       |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD23 | 20                  | 0.89     | 0.08                | 0.92       |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD22 | 20                  | 0.89     | 0.08                | 0.92       |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 20                  | 0.89     | 0.11                | 0.93       |
| (1,754) | 1:604:A:VAL:H    | 1:604:A:VAL:HG13 | 20                  | 0.79     | 0.06                | 0.8        |
| (1,754) | 1:604:A:VAL:H    | 1:604:A:VAL:HG11 | 20                  | 0.79     | 0.06                | 0.8        |
| (1,754) | 1:604:A:VAL:H    | 1:604:A:VAL:HG12 | 20                  | 0.79     | 0.06                | 0.8        |
| (1,357) | 1:608:A:VAL:HG23 | 1:629:A:VAL:HA   | 20                  | 0.75     | 0.89                | 0.4        |
| (1,357) | 1:608:A:VAL:HG21 | 1:629:A:VAL:HA   | 20                  | 0.75     | 0.89                | 0.4        |
| (1,357) | 1:608:A:VAL:HG22 | 1:629:A:VAL:HA   | 20                  | 0.75     | 0.89                | 0.4        |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 20                  | 0.75     | 0.19                | 0.74       |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 20                  | 0.75     | 0.24                | 0.68       |
| (1,332) | 1:632:A:ALA:HB1  | 1:611:A:ILE:HD11 | 20                  | 0.71     | 0.1                 | 0.68       |
| (1,332) | 1:632:A:ALA:HB1  | 1:611:A:ILE:HD12 | 20                  | 0.71     | 0.1                 | 0.68       |
| (1,332) | 1:632:A:ALA:HB2  | 1:611:A:ILE:HD11 | 20                  | 0.71     | 0.1                 | 0.68       |
| (1,332) | 1:632:A:ALA:HB2  | 1:611:A:ILE:HD13 | 20                  | 0.71     | 0.1                 | 0.68       |
| (1,332) | 1:632:A:ALA:HB3  | 1:611:A:ILE:HD13 | 20                  | 0.71     | 0.1                 | 0.68       |
| (1,332) | 1:632:A:ALA:HB1  | 1:611:A:ILE:HD13 | 20                  | 0.71     | 0.1                 | 0.68       |
| (1,332) | 1:632:A:ALA:HB3  | 1:611:A:ILE:HD11 | 20                  | 0.71     | 0.1                 | 0.68       |
| (1,332) | 1:632:A:ALA:HB2  | 1:611:A:ILE:HD12 | 20                  | 0.71     | 0.1                 | 0.68       |
| (1,332) | 1:632:A:ALA:HB3  | 1:611:A:ILE:HD12 | 20                  | 0.71     | 0.1                 | 0.68       |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 20                  | 0.71     | 0.16                | 0.76       |
| (1,411) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HB2  | 20                  | 0.71     | 0.22                | 0.77       |
| (1,411) | 1:629:A:VAL:HG11 | 1:630:A:ALA:HB2  | 20                  | 0.71     | 0.22                | 0.77       |
| (1,411) | 1:629:A:VAL:HG12 | 1:630:A:ALA:HB2  | 20                  | 0.71     | 0.22                | 0.77       |
| (1,411) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HB3  | 20                  | 0.71     | 0.22                | 0.77       |
| (1,411) | 1:629:A:VAL:HG11 | 1:630:A:ALA:HB1  | 20                  | 0.71     | 0.22                | 0.77       |
| (1,411) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HB1  | 20                  | 0.71     | 0.22                | 0.77       |
| (1,411) | 1:629:A:VAL:HG12 | 1:630:A:ALA:HB3  | 20                  | 0.71     | 0.22                | 0.77       |
| (1,411) | 1:629:A:VAL:HG12 | 1:630:A:ALA:HB1  | 20                  | 0.71     | 0.22                | 0.77       |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB2  | 20                  | 0.7      | 0.09                | 0.7        |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB1  | 20                  | 0.7      | 0.09                | 0.7        |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB3  | 20                  | 0.7      | 0.09                | 0.7        |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG12 | 20                  | 0.67     | 0.47                | 0.63       |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG13 | 20                  | 0.67     | 0.47                | 0.63       |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG11 | 20                  | 0.67     | 0.47                | 0.63       |
| (1,598) | 1:595:A:VAL:HG21 | 1:592:A:HIS:HA   | 20                  | 0.66     | 0.15                | 0.65       |
| (1,598) | 1:595:A:VAL:HG22 | 1:592:A:HIS:HA   | 20                  | 0.66     | 0.15                | 0.65       |
| (1,598) | 1:595:A:VAL:HG23 | 1:592:A:HIS:HA   | 20                  | 0.66     | 0.15                | 0.65       |
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 20                  | 0.64     | 0.05                | 0.64       |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 20                  | 0.64     | 0.05                | 0.64       |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 20                  | 0.64     | 0.05                | 0.64       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 20                  | 0.64     | 0.17                | 0.63       |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD12 | 20                  | 0.63     | 0.2                 | 0.64       |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD13 | 20                  | 0.63     | 0.2                 | 0.64       |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD11 | 20                  | 0.63     | 0.2                 | 0.64       |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG21 | 20                  | 0.63     | 0.04                | 0.64       |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG22 | 20                  | 0.63     | 0.04                | 0.64       |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG23 | 20                  | 0.63     | 0.04                | 0.64       |
| (1,396) | 1:664:A:LEU:HD23 | 1:664:A:LEU:HB2  | 20                  | 0.63     | 0.06                | 0.64       |
| (1,396) | 1:664:A:LEU:HD22 | 1:664:A:LEU:HB2  | 20                  | 0.63     | 0.06                | 0.64       |
| (1,396) | 1:664:A:LEU:HD21 | 1:664:A:LEU:HB2  | 20                  | 0.63     | 0.06                | 0.64       |
| (1,290) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 20                  | 0.58     | 0.22                | 0.68       |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB1  | 20                  | 0.57     | 0.05                | 0.57       |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB3  | 20                  | 0.57     | 0.05                | 0.57       |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB2  | 20                  | 0.57     | 0.05                | 0.57       |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 20                  | 0.56     | 0.07                | 0.56       |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 20                  | 0.54     | 0.47                | 0.3        |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG22 | 20                  | 0.52     | 0.11                | 0.51       |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG21 | 20                  | 0.52     | 0.11                | 0.51       |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG23 | 20                  | 0.52     | 0.11                | 0.51       |
| (1,200) | 1:619:A:ALA:HB1  | 1:620:A:LEU:HA   | 20                  | 0.52     | 0.01                | 0.52       |
| (1,200) | 1:619:A:ALA:HB3  | 1:620:A:LEU:HA   | 20                  | 0.52     | 0.01                | 0.52       |
| (1,200) | 1:619:A:ALA:HB2  | 1:620:A:LEU:HA   | 20                  | 0.52     | 0.01                | 0.52       |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 20                  | 0.52     | 0.05                | 0.51       |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 20                  | 0.51     | 0.01                | 0.51       |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 20                  | 0.5      | 0.04                | 0.52       |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 20                  | 0.49     | 0.08                | 0.48       |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB1  | 20                  | 0.48     | 0.02                | 0.47       |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB2  | 20                  | 0.48     | 0.02                | 0.47       |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB3  | 20                  | 0.48     | 0.02                | 0.47       |
| (1,711) | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 20                  | 0.47     | 0.2                 | 0.44       |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD11 | 20                  | 0.46     | 0.17                | 0.49       |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD12 | 20                  | 0.46     | 0.17                | 0.49       |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD13 | 20                  | 0.46     | 0.17                | 0.49       |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG22 | 20                  | 0.45     | 0.1                 | 0.44       |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG23 | 20                  | 0.45     | 0.1                 | 0.44       |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG21 | 20                  | 0.45     | 0.1                 | 0.44       |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG22 | 20                  | 0.45     | 0.05                | 0.43       |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG23 | 20                  | 0.45     | 0.05                | 0.43       |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG21 | 20                  | 0.45     | 0.05                | 0.43       |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG23 | 20                  | 0.45     | 0.1                 | 0.46       |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG22 | 20                  | 0.45     | 0.1                 | 0.46       |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG21 | 20                  | 0.45     | 0.1                 | 0.46       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD12 | 20                  | 0.44     | 0.21                | 0.42       |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD13 | 20                  | 0.44     | 0.21                | 0.42       |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD11 | 20                  | 0.44     | 0.21                | 0.42       |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 20                  | 0.43     | 0.44                | 0.24       |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 20                  | 0.43     | 0.02                | 0.43       |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 20                  | 0.42     | 0.01                | 0.42       |
| (1,942) | 1:664:A:LEU:H    | 1:664:A:LEU:HD11 | 20                  | 0.42     | 0.19                | 0.38       |
| (1,942) | 1:664:A:LEU:H    | 1:664:A:LEU:HD12 | 20                  | 0.42     | 0.19                | 0.38       |
| (1,942) | 1:664:A:LEU:H    | 1:664:A:LEU:HD13 | 20                  | 0.42     | 0.19                | 0.38       |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB3  | 20                  | 0.42     | 0.05                | 0.42       |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB2  | 20                  | 0.42     | 0.05                | 0.42       |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB1  | 20                  | 0.42     | 0.05                | 0.42       |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 20                  | 0.4      | 0.15                | 0.3        |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 20                  | 0.39     | 0.05                | 0.38       |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 20                  | 0.39     | 0.01                | 0.39       |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG23 | 20                  | 0.36     | 0.09                | 0.38       |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG21 | 20                  | 0.36     | 0.09                | 0.38       |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG22 | 20                  | 0.36     | 0.09                | 0.38       |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 20                  | 0.35     | 0.01                | 0.35       |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 20                  | 0.32     | 0.01                | 0.32       |
| (1,936) | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 20                  | 0.28     | 0.01                | 0.29       |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 20                  | 0.28     | 0.05                | 0.29       |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 20                  | 0.28     | 0.05                | 0.29       |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 20                  | 0.28     | 0.02                | 0.28       |
| (1,864) | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 20                  | 0.28     | 0.02                | 0.28       |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 20                  | 0.26     | 0.04                | 0.25       |
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD13 | 20                  | 0.26     | 0.05                | 0.27       |
| (1,21)  | 1:664:A:LEU:HD23 | 1:664:A:LEU:HD11 | 20                  | 0.26     | 0.05                | 0.27       |
| (1,21)  | 1:664:A:LEU:HD22 | 1:664:A:LEU:HD13 | 20                  | 0.26     | 0.05                | 0.27       |
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD11 | 20                  | 0.26     | 0.05                | 0.27       |
| (1,21)  | 1:664:A:LEU:HD23 | 1:664:A:LEU:HD13 | 20                  | 0.26     | 0.05                | 0.27       |
| (1,21)  | 1:664:A:LEU:HD22 | 1:664:A:LEU:HD11 | 20                  | 0.26     | 0.05                | 0.27       |
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD12 | 20                  | 0.26     | 0.05                | 0.27       |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 20                  | 0.25     | 0.04                | 0.26       |
| (1,881) | 1:648:A:GLU:H    | 1:643:A:ALA:HB2  | 20                  | 0.25     | 0.04                | 0.25       |
| (1,881) | 1:648:A:GLU:H    | 1:643:A:ALA:HB1  | 20                  | 0.25     | 0.04                | 0.25       |
| (1,881) | 1:648:A:GLU:H    | 1:643:A:ALA:HB3  | 20                  | 0.25     | 0.04                | 0.25       |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 20                  | 0.25     | 0.03                | 0.25       |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG22 | 20                  | 0.25     | 0.06                | 0.24       |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG23 | 20                  | 0.25     | 0.06                | 0.24       |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG21 | 20                  | 0.25     | 0.06                | 0.24       |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 20                  | 0.21     | 0.02                | 0.22       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 20                  | 0.21     | 0.01                | 0.21       |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 20                  | 0.2      | 0.01                | 0.2        |
| (1,866) | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 20                  | 0.2      | 0.04                | 0.2        |
| (1,504) | 1:629:A:VAL:HG11 | 1:629:A:VAL:HG21 | 20                  | 0.19     | 0.02                | 0.19       |
| (1,504) | 1:629:A:VAL:HG11 | 1:629:A:VAL:HG23 | 20                  | 0.19     | 0.02                | 0.19       |
| (1,504) | 1:629:A:VAL:HG12 | 1:629:A:VAL:HG23 | 20                  | 0.19     | 0.02                | 0.19       |
| (1,504) | 1:629:A:VAL:HG13 | 1:629:A:VAL:HG23 | 20                  | 0.19     | 0.02                | 0.19       |
| (1,504) | 1:629:A:VAL:HG11 | 1:629:A:VAL:HG22 | 20                  | 0.19     | 0.02                | 0.19       |
| (1,504) | 1:629:A:VAL:HG12 | 1:629:A:VAL:HG22 | 20                  | 0.19     | 0.02                | 0.19       |
| (1,504) | 1:629:A:VAL:HG13 | 1:629:A:VAL:HG22 | 20                  | 0.19     | 0.02                | 0.19       |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD22 | 20                  | 0.19     | 0.03                | 0.17       |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD23 | 20                  | 0.19     | 0.03                | 0.17       |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD21 | 20                  | 0.19     | 0.03                | 0.17       |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 20                  | 0.17     | 0.02                | 0.17       |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 20                  | 0.17     | 0.02                | 0.17       |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 20                  | 0.14     | 0.02                | 0.13       |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB3  | 20                  | 0.12     | 0.01                | 0.12       |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB1  | 20                  | 0.12     | 0.01                | 0.12       |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB2  | 20                  | 0.12     | 0.01                | 0.12       |
| (1,109) | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1  | 19                  | 6.45     | 1.6                 | 6.87       |
| (1,109) | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2  | 19                  | 6.45     | 1.6                 | 6.87       |
| (1,420) | 1:635:A:VAL:HG11 | 1:634:A:LYS:HE2  | 19                  | 4.92     | 1.31                | 5.33       |
| (1,420) | 1:635:A:VAL:HG13 | 1:634:A:LYS:HE2  | 19                  | 4.92     | 1.31                | 5.33       |
| (1,420) | 1:635:A:VAL:HG12 | 1:634:A:LYS:HE2  | 19                  | 4.92     | 1.31                | 5.33       |
| (1,1)   | 1:656:A:LYS:HE2  | 1:639:A:MET:HE3  | 19                  | 4.76     | 1.78                | 4.82       |
| (1,1)   | 1:656:A:LYS:HE2  | 1:639:A:MET:HE1  | 19                  | 4.76     | 1.78                | 4.82       |
| (1,1)   | 1:656:A:LYS:HE2  | 1:639:A:MET:HE2  | 19                  | 4.76     | 1.78                | 4.82       |
| (1,434) | 1:635:A:VAL:HG23 | 1:639:A:MET:HE3  | 19                  | 3.78     | 1.81                | 4.79       |
| (1,434) | 1:635:A:VAL:HG23 | 1:639:A:MET:HE1  | 19                  | 3.78     | 1.81                | 4.79       |
| (1,434) | 1:635:A:VAL:HG21 | 1:639:A:MET:HE3  | 19                  | 3.78     | 1.81                | 4.79       |
| (1,434) | 1:635:A:VAL:HG22 | 1:639:A:MET:HE1  | 19                  | 3.78     | 1.81                | 4.79       |
| (1,434) | 1:635:A:VAL:HG23 | 1:639:A:MET:HE2  | 19                  | 3.78     | 1.81                | 4.79       |
| (1,434) | 1:635:A:VAL:HG21 | 1:639:A:MET:HE1  | 19                  | 3.78     | 1.81                | 4.79       |
| (1,434) | 1:635:A:VAL:HG22 | 1:639:A:MET:HE3  | 19                  | 3.78     | 1.81                | 4.79       |
| (1,434) | 1:635:A:VAL:HG21 | 1:639:A:MET:HE2  | 19                  | 3.78     | 1.81                | 4.79       |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD22 | 19                  | 3.32     | 0.68                | 3.4        |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD23 | 19                  | 3.32     | 0.68                | 3.4        |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD21 | 19                  | 3.32     | 0.68                | 3.4        |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG22 | 19                  | 3.17     | 0.38                | 3.09       |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG21 | 19                  | 3.17     | 0.38                | 3.09       |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG23 | 19                  | 3.17     | 0.38                | 3.09       |
| (1,524) | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD3  | 19                  | 2.66     | 1.17                | 2.88       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,524)  | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD3  | 19                  | 2.66     | 1.17                | 2.88       |
| (1,524)  | 1:595:A:VAL:HG23 | 1:646:A:ARG:HD3  | 19                  | 2.66     | 1.17                | 2.88       |
| (1,536)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD23 | 19                  | 2.53     | 1.36                | 2.24       |
| (1,536)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD22 | 19                  | 2.53     | 1.36                | 2.24       |
| (1,536)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD21 | 19                  | 2.53     | 1.36                | 2.24       |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD1  | 19                  | 2.51     | 1.36                | 2.56       |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD2  | 19                  | 2.51     | 1.36                | 2.56       |
| (1,597)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD1  | 19                  | 2.51     | 1.36                | 2.56       |
| (1,597)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD2  | 19                  | 2.51     | 1.36                | 2.56       |
| (1,597)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HD1  | 19                  | 2.51     | 1.36                | 2.56       |
| (1,597)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HD2  | 19                  | 2.51     | 1.36                | 2.56       |
| (1,171)  | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 19                  | 2.49     | 0.83                | 2.73       |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD11 | 19                  | 2.45     | 0.56                | 2.39       |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD12 | 19                  | 2.45     | 0.56                | 2.39       |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD13 | 19                  | 2.45     | 0.56                | 2.39       |
| (1,640)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD12 | 19                  | 2.38     | 1.05                | 2.3        |
| (1,640)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD11 | 19                  | 2.38     | 1.05                | 2.3        |
| (1,640)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD13 | 19                  | 2.38     | 1.05                | 2.3        |
| (1,608)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD23 | 19                  | 2.37     | 1.45                | 3.26       |
| (1,608)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD22 | 19                  | 2.37     | 1.45                | 3.26       |
| (1,608)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD21 | 19                  | 2.37     | 1.45                | 3.26       |
| (1,121)  | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE1  | 19                  | 2.17     | 0.88                | 2.04       |
| (1,121)  | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE2  | 19                  | 2.17     | 0.88                | 2.04       |
| (1,121)  | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE1  | 19                  | 2.17     | 0.88                | 2.04       |
| (1,121)  | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE2  | 19                  | 2.17     | 0.88                | 2.04       |
| (1,121)  | 1:653:A:LEU:HD12 | 1:649:A:TYR:HE1  | 19                  | 2.17     | 0.88                | 2.04       |
| (1,121)  | 1:653:A:LEU:HD12 | 1:649:A:TYR:HE2  | 19                  | 2.17     | 0.88                | 2.04       |
| (1,523)  | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD2  | 19                  | 1.93     | 0.73                | 2.07       |
| (1,523)  | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD2  | 19                  | 1.93     | 0.73                | 2.07       |
| (1,523)  | 1:595:A:VAL:HG23 | 1:646:A:ARG:HD2  | 19                  | 1.93     | 0.73                | 2.07       |
| (1,406)  | 1:635:A:VAL:HG23 | 1:656:A:LYS:HG2  | 19                  | 1.76     | 0.47                | 1.58       |
| (1,406)  | 1:635:A:VAL:HG21 | 1:656:A:LYS:HG2  | 19                  | 1.76     | 0.47                | 1.58       |
| (1,406)  | 1:635:A:VAL:HG22 | 1:656:A:LYS:HG2  | 19                  | 1.76     | 0.47                | 1.58       |
| (1,243)  | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 19                  | 1.59     | 0.49                | 1.66       |
| (1,293)  | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 19                  | 1.53     | 0.05                | 1.53       |
| (1,176)  | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB1  | 19                  | 1.44     | 1.07                | 1.32       |
| (1,176)  | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB3  | 19                  | 1.44     | 1.07                | 1.32       |
| (1,176)  | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB2  | 19                  | 1.44     | 1.07                | 1.32       |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 19                  | 1.4      | 2.06                | 0.86       |
| (1,70)   | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 19                  | 1.34     | 0.42                | 1.41       |
| (1,297)  | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 19                  | 1.29     | 0.05                | 1.29       |
| (1,584)  | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD13 | 19                  | 1.06     | 0.34                | 1.12       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD13 | 19                  | 1.06     | 0.34                | 1.12       |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD11 | 19                  | 1.06     | 0.34                | 1.12       |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD11 | 19                  | 1.06     | 0.34                | 1.12       |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD12 | 19                  | 1.06     | 0.34                | 1.12       |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD12 | 19                  | 1.06     | 0.34                | 1.12       |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 19                  | 0.96     | 0.11                | 0.98       |
| (1,933) | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 19                  | 0.91     | 0.08                | 0.9        |
| (1,613) | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 19                  | 0.9      | 0.06                | 0.89       |
| (1,452) | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 19                  | 0.8      | 0.11                | 0.85       |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD22 | 19                  | 0.73     | 0.54                | 0.6        |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD23 | 19                  | 0.73     | 0.54                | 0.6        |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD21 | 19                  | 0.73     | 0.54                | 0.6        |
| (1,47)  | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 19                  | 0.61     | 0.01                | 0.62       |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 19                  | 0.57     | 0.26                | 0.61       |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 19                  | 0.57     | 0.26                | 0.61       |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 19                  | 0.57     | 0.26                | 0.61       |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 19                  | 0.57     | 0.26                | 0.61       |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 19                  | 0.57     | 0.26                | 0.61       |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 19                  | 0.57     | 0.26                | 0.61       |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 19                  | 0.53     | 0.18                | 0.63       |
| (1,358) | 1:620:A:LEU:HD23 | 1:620:A:LEU:HB2  | 19                  | 0.49     | 0.04                | 0.5        |
| (1,358) | 1:620:A:LEU:HD21 | 1:620:A:LEU:HB2  | 19                  | 0.49     | 0.04                | 0.5        |
| (1,358) | 1:620:A:LEU:HD22 | 1:620:A:LEU:HB2  | 19                  | 0.49     | 0.04                | 0.5        |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG22 | 19                  | 0.49     | 0.19                | 0.49       |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG23 | 19                  | 0.49     | 0.19                | 0.49       |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG21 | 19                  | 0.49     | 0.19                | 0.49       |
| (1,951) | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 19                  | 0.49     | 0.34                | 0.42       |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 19                  | 0.48     | 0.2                 | 0.56       |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 19                  | 0.47     | 0.26                | 0.3        |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG22 | 19                  | 0.46     | 0.09                | 0.47       |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG21 | 19                  | 0.46     | 0.09                | 0.47       |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG23 | 19                  | 0.46     | 0.09                | 0.47       |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 19                  | 0.45     | 0.05                | 0.46       |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 19                  | 0.4      | 0.05                | 0.4        |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 19                  | 0.4      | 0.07                | 0.42       |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 19                  | 0.37     | 0.02                | 0.37       |
| (1,225) | 1:632:A:ALA:HB2  | 1:604:A:VAL:HG21 | 19                  | 0.37     | 0.14                | 0.38       |
| (1,225) | 1:632:A:ALA:HB3  | 1:604:A:VAL:HG23 | 19                  | 0.37     | 0.14                | 0.38       |
| (1,225) | 1:632:A:ALA:HB2  | 1:604:A:VAL:HG22 | 19                  | 0.37     | 0.14                | 0.38       |
| (1,225) | 1:632:A:ALA:HB3  | 1:604:A:VAL:HG21 | 19                  | 0.37     | 0.14                | 0.38       |
| (1,225) | 1:632:A:ALA:HB1  | 1:604:A:VAL:HG21 | 19                  | 0.37     | 0.14                | 0.38       |
| (1,225) | 1:632:A:ALA:HB1  | 1:604:A:VAL:HG22 | 19                  | 0.37     | 0.14                | 0.38       |

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| Key     | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,225) | 1:632:A:ALA:HB3 | 1:604:A:VAL:HG22 | 19                  | 0.37     | 0.14                | 0.38       |
| (1,225) | 1:632:A:ALA:HB1 | 1:604:A:VAL:HG23 | 19                  | 0.37     | 0.14                | 0.38       |
| (1,572) | 1:654:A:ALA:HB2 | 1:657:A:ILE:HD11 | 19                  | 0.36     | 0.15                | 0.33       |
| (1,572) | 1:654:A:ALA:HB1 | 1:657:A:ILE:HD12 | 19                  | 0.36     | 0.15                | 0.33       |
| (1,572) | 1:654:A:ALA:HB2 | 1:657:A:ILE:HD12 | 19                  | 0.36     | 0.15                | 0.33       |
| (1,572) | 1:654:A:ALA:HB2 | 1:657:A:ILE:HD13 | 19                  | 0.36     | 0.15                | 0.33       |
| (1,572) | 1:654:A:ALA:HB3 | 1:657:A:ILE:HD13 | 19                  | 0.36     | 0.15                | 0.33       |
| (1,572) | 1:654:A:ALA:HB3 | 1:657:A:ILE:HD11 | 19                  | 0.36     | 0.15                | 0.33       |
| (1,572) | 1:654:A:ALA:HB3 | 1:657:A:ILE:HD12 | 19                  | 0.36     | 0.15                | 0.33       |
| (1,572) | 1:654:A:ALA:HB1 | 1:657:A:ILE:HD11 | 19                  | 0.36     | 0.15                | 0.33       |
| (1,572) | 1:654:A:ALA:HB1 | 1:657:A:ILE:HD13 | 19                  | 0.36     | 0.15                | 0.33       |
| (1,931) | 1:662:A:LYS:H   | 1:661:A:GLN:HB3  | 19                  | 0.34     | 0.04                | 0.35       |
| (1,295) | 1:633:A:LYS:HA  | 1:604:A:VAL:HG12 | 19                  | 0.32     | 0.2                 | 0.27       |
| (1,295) | 1:633:A:LYS:HA  | 1:604:A:VAL:HG11 | 19                  | 0.32     | 0.2                 | 0.27       |
| (1,295) | 1:633:A:LYS:HA  | 1:604:A:VAL:HG13 | 19                  | 0.32     | 0.2                 | 0.27       |
| (1,937) | 1:663:A:GLU:H   | 1:662:A:LYS:HB2  | 19                  | 0.31     | 0.06                | 0.31       |
| (1,279) | 1:668:A:ARG:HA  | 1:668:A:ARG:HB2  | 19                  | 0.31     | 0.01                | 0.3        |
| (1,723) | 1:609:A:GLN:H   | 1:608:A:VAL:HG11 | 19                  | 0.29     | 0.2                 | 0.24       |
| (1,723) | 1:609:A:GLN:H   | 1:608:A:VAL:HG12 | 19                  | 0.29     | 0.2                 | 0.24       |
| (1,723) | 1:609:A:GLN:H   | 1:608:A:VAL:HG13 | 19                  | 0.29     | 0.2                 | 0.24       |
| (1,428) | 1:661:A:GLN:HA  | 1:661:A:GLN:HG3  | 19                  | 0.28     | 0.22                | 0.22       |
| (1,246) | 1:659:A:LYS:HE2 | 1:659:A:LYS:HD3  | 19                  | 0.26     | 0.17                | 0.2        |
| (1,979) | 1:612:A:PHE:H   | 1:612:A:PHE:HD1  | 19                  | 0.24     | 0.04                | 0.24       |
| (1,979) | 1:612:A:PHE:H   | 1:612:A:PHE:HD2  | 19                  | 0.24     | 0.04                | 0.24       |
| (1,966) | 1:661:A:GLN:H   | 1:660:A:ILE:HG22 | 19                  | 0.2      | 0.05                | 0.2        |
| (1,966) | 1:661:A:GLN:H   | 1:660:A:ILE:HG23 | 19                  | 0.2      | 0.05                | 0.2        |
| (1,966) | 1:661:A:GLN:H   | 1:660:A:ILE:HG21 | 19                  | 0.2      | 0.05                | 0.2        |
| (1,785) | 1:616:A:ASP:H   | 1:615:A:PRO:HB3  | 19                  | 0.17     | 0.03                | 0.17       |
| (1,907) | 1:661:A:GLN:H   | 1:661:A:GLN:HB3  | 19                  | 0.14     | 0.02                | 0.14       |
| (1,912) | 1:657:A:ILE:H   | 1:655:A:GLU:HA   | 19                  | 0.14     | 0.03                | 0.13       |
| (1,181) | 1:621:A:LYS:HB2 | 1:621:A:LYS:HA   | 19                  | 0.14     | 0.01                | 0.14       |
| (1,749) | 1:602:A:HIS:H   | 1:602:A:HIS:HB3  | 19                  | 0.13     | 0.02                | 0.13       |
| (1,605) | 1:602:A:HIS:HD2 | 1:599:A:LEU:HD23 | 18                  | 4.5      | 1.94                | 5.84       |
| (1,605) | 1:602:A:HIS:HD2 | 1:599:A:LEU:HD21 | 18                  | 4.5      | 1.94                | 5.84       |
| (1,605) | 1:602:A:HIS:HD2 | 1:599:A:LEU:HD22 | 18                  | 4.5      | 1.94                | 5.84       |
| (1,594) | 1:634:A:LYS:HG2 | 1:635:A:VAL:HG11 | 18                  | 2.94     | 1.19                | 3.07       |
| (1,594) | 1:634:A:LYS:HG2 | 1:635:A:VAL:HG13 | 18                  | 2.94     | 1.19                | 3.07       |
| (1,594) | 1:634:A:LYS:HG2 | 1:635:A:VAL:HG12 | 18                  | 2.94     | 1.19                | 3.07       |
| (1,534) | 1:639:A:MET:HG2 | 1:653:A:LEU:HD22 | 18                  | 2.78     | 1.01                | 2.98       |
| (1,534) | 1:639:A:MET:HG2 | 1:653:A:LEU:HD23 | 18                  | 2.78     | 1.01                | 2.98       |
| (1,534) | 1:639:A:MET:HG2 | 1:653:A:LEU:HD21 | 18                  | 2.78     | 1.01                | 2.98       |
| (1,535) | 1:639:A:MET:HG3 | 1:653:A:LEU:HD22 | 18                  | 2.66     | 1.13                | 2.71       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,535)  | 1:639:A:MET:HG3  | 1:653:A:LEU:HD23 | 18                  | 2.66     | 1.13                | 2.71       |
| (1,535)  | 1:639:A:MET:HG3  | 1:653:A:LEU:HD21 | 18                  | 2.66     | 1.13                | 2.71       |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 18                  | 2.47     | 0.42                | 2.64       |
| (1,492)  | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 18                  | 2.4      | 0.87                | 2.38       |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 18                  | 2.3      | 0.43                | 2.41       |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 18                  | 2.3      | 0.43                | 2.41       |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 18                  | 2.3      | 0.43                | 2.41       |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 18                  | 2.3      | 0.43                | 2.41       |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 18                  | 2.3      | 0.43                | 2.41       |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 18                  | 2.3      | 0.43                | 2.41       |
| (1,623)  | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD12 | 18                  | 2.09     | 0.39                | 2.11       |
| (1,623)  | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD11 | 18                  | 2.09     | 0.39                | 2.11       |
| (1,623)  | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD13 | 18                  | 2.09     | 0.39                | 2.11       |
| (1,659)  | 1:652:A:LEU:HB3  | 1:639:A:MET:HE1  | 18                  | 2.08     | 0.82                | 2.39       |
| (1,659)  | 1:652:A:LEU:HB3  | 1:639:A:MET:HE3  | 18                  | 2.08     | 0.82                | 2.39       |
| (1,659)  | 1:652:A:LEU:HB3  | 1:639:A:MET:HE2  | 18                  | 2.08     | 0.82                | 2.39       |
| (1,24)   | 1:650:A:TYR:HA   | 1:653:A:LEU:HD11 | 18                  | 1.89     | 0.77                | 1.84       |
| (1,24)   | 1:650:A:TYR:HA   | 1:653:A:LEU:HD13 | 18                  | 1.89     | 0.77                | 1.84       |
| (1,24)   | 1:650:A:TYR:HA   | 1:653:A:LEU:HD12 | 18                  | 1.89     | 0.77                | 1.84       |
| (2,75)   | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 18                  | 1.83     | 0.27                | 1.82       |
| (2,75)   | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 18                  | 1.83     | 0.27                | 1.82       |
| (2,75)   | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 18                  | 1.83     | 0.27                | 1.82       |
| (2,75)   | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 18                  | 1.83     | 0.27                | 1.82       |
| (2,75)   | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 18                  | 1.83     | 0.27                | 1.82       |
| (2,75)   | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 18                  | 1.83     | 0.27                | 1.82       |
| (1,432)  | 1:653:A:LEU:HG   | 1:639:A:MET:HE3  | 18                  | 1.48     | 0.3                 | 1.52       |
| (1,432)  | 1:653:A:LEU:HG   | 1:639:A:MET:HE2  | 18                  | 1.48     | 0.3                 | 1.52       |
| (1,432)  | 1:653:A:LEU:HG   | 1:639:A:MET:HE1  | 18                  | 1.48     | 0.3                 | 1.52       |
| (1,624)  | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD12 | 18                  | 1.41     | 0.78                | 1.31       |
| (1,624)  | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD12 | 18                  | 1.41     | 0.78                | 1.31       |
| (1,624)  | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD11 | 18                  | 1.41     | 0.78                | 1.31       |
| (1,624)  | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD11 | 18                  | 1.41     | 0.78                | 1.31       |
| (1,624)  | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD13 | 18                  | 1.41     | 0.78                | 1.31       |
| (1,624)  | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD13 | 18                  | 1.41     | 0.78                | 1.31       |
| (1,621)  | 1:628:A:LEU:HD12 | 1:628:A:LEU:HA   | 18                  | 1.34     | 0.14                | 1.38       |
| (1,621)  | 1:628:A:LEU:HD11 | 1:628:A:LEU:HA   | 18                  | 1.34     | 0.14                | 1.38       |
| (1,621)  | 1:628:A:LEU:HD13 | 1:628:A:LEU:HA   | 18                  | 1.34     | 0.14                | 1.38       |
| (1,636)  | 1:639:A:MET:HE2  | 1:639:A:MET:HA   | 18                  | 0.85     | 0.24                | 0.79       |
| (1,636)  | 1:639:A:MET:HE3  | 1:639:A:MET:HA   | 18                  | 0.85     | 0.24                | 0.79       |
| (1,636)  | 1:639:A:MET:HE1  | 1:639:A:MET:HA   | 18                  | 0.85     | 0.24                | 0.79       |
| (1,650)  | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 18                  | 0.69     | 0.4                 | 0.72       |
| (1,354)  | 1:660:A:ILE:HD11 | 1:657:A:ILE:HA   | 18                  | 0.65     | 0.17                | 0.66       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,354) | 1:660:A:ILE:HD13 | 1:657:A:ILE:HA   | 18                  | 0.65     | 0.17                | 0.66       |
| (1,354) | 1:660:A:ILE:HD12 | 1:657:A:ILE:HA   | 18                  | 0.65     | 0.17                | 0.66       |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG23 | 18                  | 0.61     | 0.25                | 0.69       |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG22 | 18                  | 0.61     | 0.25                | 0.69       |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG21 | 18                  | 0.61     | 0.25                | 0.69       |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 18                  | 0.6      | 0.16                | 0.57       |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 18                  | 0.6      | 0.16                | 0.57       |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 18                  | 0.6      | 0.16                | 0.57       |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 18                  | 0.6      | 0.16                | 0.57       |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 18                  | 0.6      | 0.16                | 0.57       |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 18                  | 0.6      | 0.16                | 0.57       |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 18                  | 0.54     | 0.46                | 0.34       |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 18                  | 0.54     | 0.46                | 0.34       |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 18                  | 0.54     | 0.46                | 0.34       |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 18                  | 0.54     | 0.46                | 0.34       |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 18                  | 0.54     | 0.46                | 0.34       |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 18                  | 0.54     | 0.46                | 0.34       |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 18                  | 0.54     | 0.46                | 0.34       |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 18                  | 0.54     | 0.46                | 0.34       |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 18                  | 0.54     | 0.46                | 0.34       |
| (1,457) | 1:608:A:VAL:HG22 | 1:605:A:HIS:HA   | 18                  | 0.52     | 0.27                | 0.48       |
| (1,457) | 1:608:A:VAL:HG23 | 1:605:A:HIS:HA   | 18                  | 0.52     | 0.27                | 0.48       |
| (1,457) | 1:608:A:VAL:HG21 | 1:605:A:HIS:HA   | 18                  | 0.52     | 0.27                | 0.48       |
| (1,986) | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 18                  | 0.49     | 0.21                | 0.46       |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 18                  | 0.48     | 0.21                | 0.39       |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD11 | 18                  | 0.41     | 0.07                | 0.42       |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD13 | 18                  | 0.41     | 0.07                | 0.42       |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD12 | 18                  | 0.41     | 0.07                | 0.42       |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 18                  | 0.39     | 0.01                | 0.39       |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 18                  | 0.38     | 0.02                | 0.38       |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 18                  | 0.38     | 0.02                | 0.38       |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 18                  | 0.38     | 0.02                | 0.38       |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 18                  | 0.35     | 0.02                | 0.35       |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 18                  | 0.28     | 0.02                | 0.28       |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 18                  | 0.28     | 0.02                | 0.28       |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 18                  | 0.28     | 0.02                | 0.28       |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 18                  | 0.23     | 0.01                | 0.23       |
| (1,223) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HA   | 18                  | 0.22     | 0.11                | 0.18       |
| (1,223) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HA   | 18                  | 0.22     | 0.11                | 0.18       |
| (1,223) | 1:604:A:VAL:HG11 | 1:604:A:VAL:HA   | 18                  | 0.22     | 0.11                | 0.18       |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 18                  | 0.18     | 0.04                | 0.18       |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 18                  | 0.17     | 0.05                | 0.16       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 18                  | 0.17     | 0.01                | 0.17       |
| (1,141) | 1:595:A:VAL:HG23 | 1:640:A:TYR:HE1  | 17                  | 3.63     | 2.13                | 2.52       |
| (1,141) | 1:595:A:VAL:HG23 | 1:640:A:TYR:HE2  | 17                  | 3.63     | 2.13                | 2.52       |
| (1,141) | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE1  | 17                  | 3.63     | 2.13                | 2.52       |
| (1,141) | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE2  | 17                  | 3.63     | 2.13                | 2.52       |
| (1,141) | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE1  | 17                  | 3.63     | 2.13                | 2.52       |
| (1,141) | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE2  | 17                  | 3.63     | 2.13                | 2.52       |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 17                  | 3.16     | 2.18                | 1.75       |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 17                  | 3.16     | 2.18                | 1.75       |
| (1,142) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE1  | 17                  | 3.14     | 1.93                | 2.29       |
| (1,142) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE2  | 17                  | 3.14     | 1.93                | 2.29       |
| (1,142) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HE1  | 17                  | 3.14     | 1.93                | 2.29       |
| (1,142) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HE2  | 17                  | 3.14     | 1.93                | 2.29       |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE1  | 17                  | 3.14     | 1.93                | 2.29       |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE2  | 17                  | 3.14     | 1.93                | 2.29       |
| (1,617) | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 17                  | 2.15     | 0.51                | 2.08       |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD1  | 17                  | 1.98     | 0.94                | 1.61       |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD2  | 17                  | 1.98     | 0.94                | 1.61       |
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD1  | 17                  | 1.98     | 0.94                | 1.61       |
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD2  | 17                  | 1.98     | 0.94                | 1.61       |
| (1,116) | 1:653:A:LEU:HD12 | 1:650:A:TYR:HD1  | 17                  | 1.98     | 0.94                | 1.61       |
| (1,116) | 1:653:A:LEU:HD12 | 1:650:A:TYR:HD2  | 17                  | 1.98     | 0.94                | 1.61       |
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD12 | 17                  | 1.8      | 0.58                | 1.93       |
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD13 | 17                  | 1.8      | 0.58                | 1.93       |
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD11 | 17                  | 1.8      | 0.58                | 1.93       |
| (1,601) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD1  | 17                  | 1.63     | 1.18                | 0.85       |
| (1,601) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD2  | 17                  | 1.63     | 1.18                | 0.85       |
| (1,601) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HD1  | 17                  | 1.63     | 1.18                | 0.85       |
| (1,601) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HD2  | 17                  | 1.63     | 1.18                | 0.85       |
| (1,601) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HD1  | 17                  | 1.63     | 1.18                | 0.85       |
| (1,601) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HD2  | 17                  | 1.63     | 1.18                | 0.85       |
| (1,74)  | 1:672:A:LEU:HD13 | 1:672:A:LEU:HA   | 17                  | 1.61     | 0.05                | 1.62       |
| (1,74)  | 1:672:A:LEU:HD12 | 1:672:A:LEU:HA   | 17                  | 1.61     | 0.05                | 1.62       |
| (1,74)  | 1:672:A:LEU:HD11 | 1:672:A:LEU:HA   | 17                  | 1.61     | 0.05                | 1.62       |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD22 | 17                  | 1.59     | 0.33                | 1.61       |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD21 | 17                  | 1.59     | 0.33                | 1.61       |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD23 | 17                  | 1.59     | 0.33                | 1.61       |
| (1,394) | 1:635:A:VAL:HG13 | 1:632:A:ALA:HA   | 17                  | 1.53     | 0.61                | 1.84       |
| (1,394) | 1:635:A:VAL:HG12 | 1:632:A:ALA:HA   | 17                  | 1.53     | 0.61                | 1.84       |
| (1,394) | 1:635:A:VAL:HG11 | 1:632:A:ALA:HA   | 17                  | 1.53     | 0.61                | 1.84       |
| (1,484) | 1:607:A:LEU:HD22 | 1:653:A:LEU:HB2  | 17                  | 1.52     | 0.72                | 1.24       |
| (1,484) | 1:607:A:LEU:HD23 | 1:653:A:LEU:HB2  | 17                  | 1.52     | 0.72                | 1.24       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,484) | 1:607:A:LEU:HD21 | 1:653:A:LEU:HB2  | 17                  | 1.52     | 0.72                | 1.24       |
| (1,366) | 1:639:A:MET:HE3  | 1:653:A:LEU:HD23 | 17                  | 1.11     | 0.51                | 1.09       |
| (1,366) | 1:639:A:MET:HE2  | 1:653:A:LEU:HD23 | 17                  | 1.11     | 0.51                | 1.09       |
| (1,366) | 1:639:A:MET:HE1  | 1:653:A:LEU:HD23 | 17                  | 1.11     | 0.51                | 1.09       |
| (1,366) | 1:639:A:MET:HE1  | 1:653:A:LEU:HD21 | 17                  | 1.11     | 0.51                | 1.09       |
| (1,366) | 1:639:A:MET:HE3  | 1:653:A:LEU:HD22 | 17                  | 1.11     | 0.51                | 1.09       |
| (1,366) | 1:639:A:MET:HE2  | 1:653:A:LEU:HD21 | 17                  | 1.11     | 0.51                | 1.09       |
| (1,366) | 1:639:A:MET:HE3  | 1:653:A:LEU:HD21 | 17                  | 1.11     | 0.51                | 1.09       |
| (1,366) | 1:639:A:MET:HE1  | 1:653:A:LEU:HD22 | 17                  | 1.11     | 0.51                | 1.09       |
| (1,366) | 1:639:A:MET:HE2  | 1:653:A:LEU:HD22 | 17                  | 1.11     | 0.51                | 1.09       |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 17                  | 0.7      | 0.28                | 0.58       |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 17                  | 0.68     | 0.21                | 0.68       |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 17                  | 0.68     | 0.21                | 0.68       |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 17                  | 0.55     | 0.08                | 0.57       |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 17                  | 0.44     | 0.16                | 0.43       |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 17                  | 0.44     | 0.16                | 0.43       |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 17                  | 0.44     | 0.16                | 0.43       |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 17                  | 0.44     | 0.16                | 0.43       |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 17                  | 0.44     | 0.16                | 0.43       |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 17                  | 0.44     | 0.16                | 0.43       |
| (1,657) | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE1  | 17                  | 0.33     | 0.16                | 0.33       |
| (1,657) | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE2  | 17                  | 0.33     | 0.16                | 0.33       |
| (1,657) | 1:595:A:VAL:HG12 | 1:649:A:TYR:HE1  | 17                  | 0.33     | 0.16                | 0.33       |
| (1,657) | 1:595:A:VAL:HG12 | 1:649:A:TYR:HE2  | 17                  | 0.33     | 0.16                | 0.33       |
| (1,657) | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE1  | 17                  | 0.33     | 0.16                | 0.33       |
| (1,657) | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE2  | 17                  | 0.33     | 0.16                | 0.33       |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG11 | 17                  | 0.32     | 0.09                | 0.32       |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG12 | 17                  | 0.32     | 0.09                | 0.32       |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG13 | 17                  | 0.32     | 0.09                | 0.32       |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 17                  | 0.3      | 0.01                | 0.3        |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 17                  | 0.27     | 0.03                | 0.28       |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 17                  | 0.27     | 0.03                | 0.28       |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 17                  | 0.27     | 0.03                | 0.28       |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 17                  | 0.25     | 0.05                | 0.26       |
| (2,143) | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 17                  | 0.19     | 0.05                | 0.19       |
| (2,143) | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 17                  | 0.19     | 0.05                | 0.19       |
| (2,143) | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 17                  | 0.19     | 0.05                | 0.19       |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 17                  | 0.15     | 0.04                | 0.14       |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 17                  | 0.15     | 0.04                | 0.14       |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 17                  | 0.15     | 0.04                | 0.14       |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 17                  | 0.15     | 0.02                | 0.16       |
| (1,470) | 1:635:A:VAL:HG12 | 1:639:A:MET:HE3  | 16                  | 1.72     | 1.25                | 1.35       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,470) | 1:635:A:VAL:HG11 | 1:639:A:MET:HE1  | 16                  | 1.72     | 1.25                | 1.35       |
| (1,470) | 1:635:A:VAL:HG11 | 1:639:A:MET:HE3  | 16                  | 1.72     | 1.25                | 1.35       |
| (1,470) | 1:635:A:VAL:HG11 | 1:639:A:MET:HE2  | 16                  | 1.72     | 1.25                | 1.35       |
| (1,470) | 1:635:A:VAL:HG12 | 1:639:A:MET:HE2  | 16                  | 1.72     | 1.25                | 1.35       |
| (1,470) | 1:635:A:VAL:HG13 | 1:639:A:MET:HE3  | 16                  | 1.72     | 1.25                | 1.35       |
| (1,470) | 1:635:A:VAL:HG13 | 1:639:A:MET:HE1  | 16                  | 1.72     | 1.25                | 1.35       |
| (1,470) | 1:635:A:VAL:HG13 | 1:639:A:MET:HE2  | 16                  | 1.72     | 1.25                | 1.35       |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE1  | 16                  | 1.59     | 0.3                 | 1.52       |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE2  | 16                  | 1.59     | 0.3                 | 1.52       |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE3  | 16                  | 1.59     | 0.3                 | 1.52       |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 16                  | 1.53     | 0.33                | 1.67       |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 16                  | 1.48     | 0.04                | 1.49       |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 16                  | 1.41     | 0.33                | 1.42       |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 16                  | 1.23     | 0.46                | 1.46       |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 16                  | 1.1      | 0.77                | 1.12       |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 16                  | 1.1      | 0.77                | 1.12       |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 16                  | 1.1      | 0.77                | 1.12       |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD1  | 16                  | 1.0      | 0.86                | 0.7        |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD2  | 16                  | 1.0      | 0.86                | 0.7        |
| (1,117) | 1:653:A:LEU:HD21 | 1:650:A:TYR:HD1  | 16                  | 1.0      | 0.86                | 0.7        |
| (1,117) | 1:653:A:LEU:HD21 | 1:650:A:TYR:HD2  | 16                  | 1.0      | 0.86                | 0.7        |
| (1,117) | 1:653:A:LEU:HD22 | 1:650:A:TYR:HD1  | 16                  | 1.0      | 0.86                | 0.7        |
| (1,117) | 1:653:A:LEU:HD22 | 1:650:A:TYR:HD2  | 16                  | 1.0      | 0.86                | 0.7        |
| (1,167) | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 16                  | 0.95     | 0.22                | 1.02       |
| (1,654) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 16                  | 0.94     | 0.13                | 0.9        |
| (1,971) | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 16                  | 0.83     | 0.15                | 0.86       |
| (1,214) | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD11 | 16                  | 0.77     | 0.3                 | 0.8        |
| (1,214) | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD13 | 16                  | 0.77     | 0.3                 | 0.8        |
| (1,214) | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD12 | 16                  | 0.77     | 0.3                 | 0.8        |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 16                  | 0.31     | 0.15                | 0.24       |
| (2,93)  | 2:534:B:PHE:HD1  | 2:534:B:PHE:HB3  | 16                  | 0.3      | 0.06                | 0.33       |
| (2,93)  | 2:534:B:PHE:HD2  | 2:534:B:PHE:HB3  | 16                  | 0.3      | 0.06                | 0.33       |
| (1,915) | 1:657:A:ILE:H    | 1:657:A:ILE:HD11 | 16                  | 0.27     | 0.12                | 0.24       |
| (1,915) | 1:657:A:ILE:H    | 1:657:A:ILE:HD12 | 16                  | 0.27     | 0.12                | 0.24       |
| (1,915) | 1:657:A:ILE:H    | 1:657:A:ILE:HD13 | 16                  | 0.27     | 0.12                | 0.24       |
| (1,402) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HA   | 16                  | 0.25     | 0.07                | 0.24       |
| (1,402) | 1:629:A:VAL:HG11 | 1:630:A:ALA:HA   | 16                  | 0.25     | 0.07                | 0.24       |
| (1,402) | 1:629:A:VAL:HG12 | 1:630:A:ALA:HA   | 16                  | 0.25     | 0.07                | 0.24       |
| (1,688) | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 16                  | 0.24     | 0.02                | 0.25       |
| (1,582) | 1:599:A:LEU:HD21 | 1:599:A:LEU:HD13 | 16                  | 0.21     | 0.04                | 0.21       |
| (1,582) | 1:599:A:LEU:HD21 | 1:599:A:LEU:HD12 | 16                  | 0.21     | 0.04                | 0.21       |
| (1,582) | 1:599:A:LEU:HD23 | 1:599:A:LEU:HD11 | 16                  | 0.21     | 0.04                | 0.21       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,582)  | 1:599:A:LEU:HD23 | 1:599:A:LEU:HD13 | 16                  | 0.21     | 0.04                | 0.21       |
| (1,582)  | 1:599:A:LEU:HD22 | 1:599:A:LEU:HD11 | 16                  | 0.21     | 0.04                | 0.21       |
| (1,582)  | 1:599:A:LEU:HD22 | 1:599:A:LEU:HD12 | 16                  | 0.21     | 0.04                | 0.21       |
| (1,582)  | 1:599:A:LEU:HD22 | 1:599:A:LEU:HD13 | 16                  | 0.21     | 0.04                | 0.21       |
| (1,582)  | 1:599:A:LEU:HD23 | 1:599:A:LEU:HD12 | 16                  | 0.21     | 0.04                | 0.21       |
| (1,409)  | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 16                  | 0.19     | 0.07                | 0.16       |
| (1,191)  | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 16                  | 0.19     | 0.05                | 0.18       |
| (2,183)  | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 16                  | 0.18     | 0.02                | 0.19       |
| (1,694)  | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 16                  | 0.17     | 0.01                | 0.17       |
| (1,963)  | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 16                  | 0.12     | 0.01                | 0.12       |
| (1,480)  | 1:653:A:LEU:HD23 | 1:636:A:GLU:HA   | 15                  | 2.29     | 0.89                | 2.59       |
| (1,480)  | 1:653:A:LEU:HD22 | 1:636:A:GLU:HA   | 15                  | 2.29     | 0.89                | 2.59       |
| (1,480)  | 1:653:A:LEU:HD21 | 1:636:A:GLU:HA   | 15                  | 2.29     | 0.89                | 2.59       |
| (1,219)  | 1:604:A:VAL:HA   | 1:607:A:LEU:HD21 | 15                  | 1.53     | 0.98                | 2.14       |
| (1,219)  | 1:604:A:VAL:HA   | 1:607:A:LEU:HD22 | 15                  | 1.53     | 0.98                | 2.14       |
| (1,219)  | 1:604:A:VAL:HA   | 1:607:A:LEU:HD23 | 15                  | 1.53     | 0.98                | 2.14       |
| (1,857)  | 1:636:A:GLU:H    | 1:635:A:VAL:HG21 | 15                  | 0.94     | 0.16                | 0.91       |
| (1,857)  | 1:636:A:GLU:H    | 1:635:A:VAL:HG22 | 15                  | 0.94     | 0.16                | 0.91       |
| (1,857)  | 1:636:A:GLU:H    | 1:635:A:VAL:HG23 | 15                  | 0.94     | 0.16                | 0.91       |
| (1,853)  | 1:635:A:VAL:H    | 1:635:A:VAL:HG12 | 15                  | 0.83     | 0.23                | 0.9        |
| (1,853)  | 1:635:A:VAL:H    | 1:635:A:VAL:HG11 | 15                  | 0.83     | 0.23                | 0.9        |
| (1,853)  | 1:635:A:VAL:H    | 1:635:A:VAL:HG13 | 15                  | 0.83     | 0.23                | 0.9        |
| (1,270)  | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 15                  | 0.76     | 0.39                | 0.95       |
| (1,548)  | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 15                  | 0.66     | 0.25                | 0.64       |
| (1,655)  | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 15                  | 0.55     | 0.01                | 0.55       |
| (1,424)  | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 15                  | 0.5      | 0.23                | 0.41       |
| (1,247)  | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 15                  | 0.44     | 0.01                | 0.45       |
| (2,133)  | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 15                  | 0.43     | 0.08                | 0.41       |
| (2,200)  | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 15                  | 0.38     | 0.02                | 0.38       |
| (1,63)   | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 15                  | 0.32     | 0.05                | 0.31       |
| (1,520)  | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 15                  | 0.26     | 0.06                | 0.25       |
| (1,57)   | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 15                  | 0.17     | 0.01                | 0.17       |
| (1,603)  | 1:599:A:LEU:HD11 | 1:595:A:VAL:HG11 | 14                  | 1.79     | 0.75                | 2.02       |
| (1,603)  | 1:599:A:LEU:HD12 | 1:595:A:VAL:HG11 | 14                  | 1.79     | 0.75                | 2.02       |
| (1,603)  | 1:599:A:LEU:HD12 | 1:595:A:VAL:HG13 | 14                  | 1.79     | 0.75                | 2.02       |
| (1,603)  | 1:599:A:LEU:HD11 | 1:595:A:VAL:HG13 | 14                  | 1.79     | 0.75                | 2.02       |
| (1,603)  | 1:599:A:LEU:HD13 | 1:595:A:VAL:HG12 | 14                  | 1.79     | 0.75                | 2.02       |
| (1,603)  | 1:599:A:LEU:HD12 | 1:595:A:VAL:HG12 | 14                  | 1.79     | 0.75                | 2.02       |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 14                  | 1.42     | 1.14                | 1.07       |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 14                  | 1.42     | 1.14                | 1.07       |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 14                  | 1.42     | 1.14                | 1.07       |
| (1,742)  | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 14                  | 1.05     | 0.41                | 1.25       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 14                  | 1.04     | 0.08                | 1.02       |
| (2,136) | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 14                  | 0.96     | 0.24                | 1.0        |
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD11 | 14                  | 0.93     | 0.78                | 0.66       |
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD13 | 14                  | 0.93     | 0.78                | 0.66       |
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD12 | 14                  | 0.93     | 0.78                | 0.66       |
| (1,719) | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 14                  | 0.8      | 0.23                | 0.74       |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 14                  | 0.79     | 0.24                | 0.73       |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 14                  | 0.79     | 0.24                | 0.73       |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 14                  | 0.79     | 0.24                | 0.73       |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 14                  | 0.79     | 0.24                | 0.73       |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 14                  | 0.79     | 0.24                | 0.73       |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 14                  | 0.79     | 0.24                | 0.73       |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 14                  | 0.79     | 0.24                | 0.73       |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 14                  | 0.79     | 0.24                | 0.73       |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 14                  | 0.79     | 0.24                | 0.73       |
| (1,478) | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 14                  | 0.72     | 0.24                | 0.88       |
| (1,583) | 1:603:A:LEU:HD13 | 1:599:A:LEU:HD13 | 14                  | 0.62     | 0.33                | 0.57       |
| (1,583) | 1:603:A:LEU:HD11 | 1:599:A:LEU:HD11 | 14                  | 0.62     | 0.33                | 0.57       |
| (1,583) | 1:603:A:LEU:HD13 | 1:599:A:LEU:HD11 | 14                  | 0.62     | 0.33                | 0.57       |
| (1,583) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD11 | 14                  | 0.62     | 0.33                | 0.57       |
| (1,583) | 1:603:A:LEU:HD13 | 1:599:A:LEU:HD12 | 14                  | 0.62     | 0.33                | 0.57       |
| (1,583) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD12 | 14                  | 0.62     | 0.33                | 0.57       |
| (1,583) | 1:603:A:LEU:HD11 | 1:599:A:LEU:HD13 | 14                  | 0.62     | 0.33                | 0.57       |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 14                  | 0.41     | 0.17                | 0.41       |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 14                  | 0.41     | 0.17                | 0.41       |
| (1,464) | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 14                  | 0.34     | 0.32                | 0.14       |
| (1,513) | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 14                  | 0.32     | 0.24                | 0.18       |
| (1,392) | 1:635:A:VAL:HG21 | 1:632:A:ALA:HA   | 14                  | 0.32     | 0.13                | 0.33       |
| (1,392) | 1:635:A:VAL:HG22 | 1:632:A:ALA:HA   | 14                  | 0.32     | 0.13                | 0.33       |
| (1,392) | 1:635:A:VAL:HG23 | 1:632:A:ALA:HA   | 14                  | 0.32     | 0.13                | 0.33       |
| (1,952) | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 14                  | 0.19     | 0.08                | 0.15       |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 13                  | 2.7      | 1.71                | 3.57       |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 13                  | 2.7      | 1.71                | 3.57       |
| (1,6)   | 1:608:A:VAL:HG13 | 1:625:A:MET:HE3  | 13                  | 1.63     | 1.06                | 1.61       |
| (1,6)   | 1:608:A:VAL:HG13 | 1:625:A:MET:HE1  | 13                  | 1.63     | 1.06                | 1.61       |
| (1,6)   | 1:608:A:VAL:HG13 | 1:625:A:MET:HE2  | 13                  | 1.63     | 1.06                | 1.61       |
| (1,6)   | 1:608:A:VAL:HG11 | 1:625:A:MET:HE3  | 13                  | 1.63     | 1.06                | 1.61       |
| (1,495) | 1:653:A:LEU:HD11 | 1:603:A:LEU:HD13 | 13                  | 1.41     | 0.8                 | 1.16       |
| (1,495) | 1:653:A:LEU:HD11 | 1:603:A:LEU:HD11 | 13                  | 1.41     | 0.8                 | 1.16       |
| (1,495) | 1:653:A:LEU:HD13 | 1:603:A:LEU:HD13 | 13                  | 1.41     | 0.8                 | 1.16       |
| (1,495) | 1:653:A:LEU:HD13 | 1:603:A:LEU:HD12 | 13                  | 1.41     | 0.8                 | 1.16       |
| (1,495) | 1:653:A:LEU:HD12 | 1:603:A:LEU:HD12 | 13                  | 1.41     | 0.8                 | 1.16       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,495) | 1:653:A:LEU:HD12 | 1:603:A:LEU:HD13 | 13                  | 1.41     | 0.8                 | 1.16       |
| (1,495) | 1:653:A:LEU:HD12 | 1:603:A:LEU:HD11 | 13                  | 1.41     | 0.8                 | 1.16       |
| (1,106) | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 13                  | 1.37     | 0.11                | 1.41       |
| (1,71)  | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 13                  | 1.0      | 0.57                | 1.05       |
| (1,974) | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 13                  | 0.67     | 0.03                | 0.66       |
| (2,219) | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 13                  | 0.57     | 0.1                 | 0.61       |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD23 | 13                  | 0.42     | 0.17                | 0.35       |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD22 | 13                  | 0.42     | 0.17                | 0.35       |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD21 | 13                  | 0.42     | 0.17                | 0.35       |
| (1,274) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB3  | 13                  | 0.38     | 0.03                | 0.39       |
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 13                  | 0.37     | 0.0                 | 0.37       |
| (1,843) | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 13                  | 0.33     | 0.1                 | 0.35       |
| (1,349) | 1:610:A:ALA:HB1  | 1:657:A:ILE:HD12 | 13                  | 0.27     | 0.11                | 0.27       |
| (1,349) | 1:610:A:ALA:HB3  | 1:657:A:ILE:HD12 | 13                  | 0.27     | 0.11                | 0.27       |
| (1,349) | 1:610:A:ALA:HB1  | 1:657:A:ILE:HD13 | 13                  | 0.27     | 0.11                | 0.27       |
| (1,349) | 1:610:A:ALA:HB2  | 1:657:A:ILE:HD13 | 13                  | 0.27     | 0.11                | 0.27       |
| (1,349) | 1:610:A:ALA:HB2  | 1:657:A:ILE:HD11 | 13                  | 0.27     | 0.11                | 0.27       |
| (1,349) | 1:610:A:ALA:HB2  | 1:657:A:ILE:HD12 | 13                  | 0.27     | 0.11                | 0.27       |
| (1,349) | 1:610:A:ALA:HB3  | 1:657:A:ILE:HD13 | 13                  | 0.27     | 0.11                | 0.27       |
| (1,224) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HG21 | 13                  | 0.19     | 0.05                | 0.19       |
| (1,224) | 1:604:A:VAL:HG11 | 1:604:A:VAL:HG23 | 13                  | 0.19     | 0.05                | 0.19       |
| (1,224) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HG22 | 13                  | 0.19     | 0.05                | 0.19       |
| (1,224) | 1:604:A:VAL:HG11 | 1:604:A:VAL:HG22 | 13                  | 0.19     | 0.05                | 0.19       |
| (1,224) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HG22 | 13                  | 0.19     | 0.05                | 0.19       |
| (1,224) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HG23 | 13                  | 0.19     | 0.05                | 0.19       |
| (1,224) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HG23 | 13                  | 0.19     | 0.05                | 0.19       |
| (1,224) | 1:604:A:VAL:HG11 | 1:604:A:VAL:HG21 | 13                  | 0.19     | 0.05                | 0.19       |
| (1,412) | 1:630:A:ALA:HB1  | 1:627:A:ASN:HA   | 13                  | 0.18     | 0.05                | 0.17       |
| (1,412) | 1:630:A:ALA:HB3  | 1:627:A:ASN:HA   | 13                  | 0.18     | 0.05                | 0.17       |
| (1,412) | 1:630:A:ALA:HB2  | 1:627:A:ASN:HA   | 13                  | 0.18     | 0.05                | 0.17       |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 13                  | 0.18     | 0.11                | 0.13       |
| (1,489) | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 13                  | 0.12     | 0.01                | 0.12       |
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 13                  | 0.11     | 0.01                | 0.11       |
| (1,637) | 1:642:A:SER:HB2  | 1:639:A:MET:HA   | 12                  | 1.69     | 0.05                | 1.68       |
| (1,496) | 1:599:A:LEU:HD13 | 1:603:A:LEU:HD22 | 12                  | 1.51     | 0.82                | 1.49       |
| (1,496) | 1:599:A:LEU:HD11 | 1:603:A:LEU:HD23 | 12                  | 1.51     | 0.82                | 1.49       |
| (1,496) | 1:599:A:LEU:HD11 | 1:603:A:LEU:HD22 | 12                  | 1.51     | 0.82                | 1.49       |
| (1,496) | 1:599:A:LEU:HD12 | 1:603:A:LEU:HD21 | 12                  | 1.51     | 0.82                | 1.49       |
| (1,496) | 1:599:A:LEU:HD11 | 1:603:A:LEU:HD21 | 12                  | 1.51     | 0.82                | 1.49       |
| (1,496) | 1:599:A:LEU:HD13 | 1:603:A:LEU:HD23 | 12                  | 1.51     | 0.82                | 1.49       |
| (1,496) | 1:599:A:LEU:HD12 | 1:603:A:LEU:HD22 | 12                  | 1.51     | 0.82                | 1.49       |
| (1,496) | 1:599:A:LEU:HD12 | 1:603:A:LEU:HD23 | 12                  | 1.51     | 0.82                | 1.49       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE1  | 12                  | 1.38     | 0.71                | 1.4        |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE2  | 12                  | 1.38     | 0.71                | 1.4        |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE1  | 12                  | 1.38     | 0.71                | 1.4        |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE2  | 12                  | 1.38     | 0.71                | 1.4        |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE1  | 12                  | 1.38     | 0.71                | 1.4        |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE2  | 12                  | 1.38     | 0.71                | 1.4        |
| (1,571) | 1:591:A:TRP:HD1  | 1:589:A:LYS:HA   | 12                  | 1.06     | 1.4                 | 0.7        |
| (1,207) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD12 | 12                  | 0.93     | 0.51                | 0.72       |
| (1,207) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD11 | 12                  | 0.93     | 0.51                | 0.72       |
| (1,207) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD13 | 12                  | 0.93     | 0.51                | 0.72       |
| (1,211) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD13 | 12                  | 0.67     | 0.11                | 0.68       |
| (1,211) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD12 | 12                  | 0.67     | 0.11                | 0.68       |
| (1,211) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD11 | 12                  | 0.67     | 0.11                | 0.68       |
| (2,252) | 2:535:B:SER:H    | 2:534:B:PHE:HD1  | 12                  | 0.62     | 0.27                | 0.64       |
| (1,302) | 1:614:A:THR:HG21 | 1:617:A:PRO:HA   | 12                  | 0.56     | 0.33                | 0.45       |
| (1,302) | 1:614:A:THR:HG22 | 1:617:A:PRO:HA   | 12                  | 0.56     | 0.33                | 0.45       |
| (1,302) | 1:614:A:THR:HG23 | 1:617:A:PRO:HA   | 12                  | 0.56     | 0.33                | 0.45       |
| (1,209) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD22 | 12                  | 0.54     | 0.2                 | 0.64       |
| (1,209) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD23 | 12                  | 0.54     | 0.2                 | 0.64       |
| (1,209) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD21 | 12                  | 0.54     | 0.2                 | 0.64       |
| (1,36)  | 1:609:A:GLN:HA   | 1:609:A:GLN:HG3  | 12                  | 0.46     | 0.03                | 0.46       |
| (1,2)   | 1:639:A:MET:HG2  | 1:639:A:MET:HE3  | 12                  | 0.43     | 0.11                | 0.46       |
| (1,2)   | 1:639:A:MET:HG2  | 1:639:A:MET:HE2  | 12                  | 0.43     | 0.11                | 0.46       |
| (1,2)   | 1:639:A:MET:HG2  | 1:639:A:MET:HE1  | 12                  | 0.43     | 0.11                | 0.46       |
| (1,680) | 1:642:A:SER:H    | 1:642:A:SER:HB2  | 12                  | 0.42     | 0.01                | 0.42       |
| (1,903) | 1:653:A:LEU:H    | 1:653:A:LEU:HD11 | 12                  | 0.32     | 0.1                 | 0.34       |
| (1,903) | 1:653:A:LEU:H    | 1:653:A:LEU:HD12 | 12                  | 0.32     | 0.1                 | 0.34       |
| (1,903) | 1:653:A:LEU:H    | 1:653:A:LEU:HD13 | 12                  | 0.32     | 0.1                 | 0.34       |
| (2,121) | 2:540:B:MET:HA   | 2:540:B:MET:HG2  | 12                  | 0.18     | 0.03                | 0.17       |
| (2,245) | 2:537:B:ILE:H    | 2:537:B:ILE:HG12 | 12                  | 0.16     | 0.02                | 0.16       |
| (1,54)  | 1:613:A:PRO:HG3  | 1:612:A:PHE:HA   | 12                  | 0.14     | 0.02                | 0.15       |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE1  | 11                  | 2.38     | 0.97                | 3.02       |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE2  | 11                  | 2.38     | 0.97                | 3.02       |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE1  | 11                  | 2.38     | 0.97                | 3.02       |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE2  | 11                  | 2.38     | 0.97                | 3.02       |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE1  | 11                  | 2.38     | 0.97                | 3.02       |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE2  | 11                  | 2.38     | 0.97                | 3.02       |
| (1,607) | 1:599:A:LEU:HD23 | 1:602:A:HIS:HB2  | 11                  | 2.28     | 0.16                | 2.34       |
| (1,607) | 1:599:A:LEU:HD21 | 1:602:A:HIS:HB2  | 11                  | 2.28     | 0.16                | 2.34       |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD23 | 11                  | 1.56     | 0.09                | 1.54       |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD21 | 11                  | 1.56     | 0.09                | 1.54       |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD22 | 11                  | 1.56     | 0.09                | 1.54       |

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| Key     | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,787) | 1:616:A:ASP:H   | 1:614:A:THR:HG21 | 11                  | 0.66     | 0.3                 | 0.68       |
| (1,787) | 1:616:A:ASP:H   | 1:614:A:THR:HG22 | 11                  | 0.66     | 0.3                 | 0.68       |
| (1,787) | 1:616:A:ASP:H   | 1:614:A:THR:HG23 | 11                  | 0.66     | 0.3                 | 0.68       |
| (1,745) | 1:600:A:ARG:H   | 1:599:A:LEU:HB2  | 11                  | 0.59     | 0.05                | 0.6        |
| (1,453) | 1:634:A:LYS:HG2 | 1:634:A:LYS:HA   | 11                  | 0.57     | 0.08                | 0.55       |
| (1,993) | 1:619:A:ALA:HB1 | 1:612:A:PHE:HZ   | 11                  | 0.49     | 0.53                | 0.29       |
| (1,993) | 1:619:A:ALA:HB2 | 1:612:A:PHE:HZ   | 11                  | 0.49     | 0.53                | 0.29       |
| (1,993) | 1:619:A:ALA:HB3 | 1:612:A:PHE:HZ   | 11                  | 0.49     | 0.53                | 0.29       |
| (1,503) | 1:625:A:MET:HG2 | 1:629:A:VAL:HG22 | 11                  | 0.47     | 0.24                | 0.42       |
| (1,503) | 1:625:A:MET:HG2 | 1:629:A:VAL:HG21 | 11                  | 0.47     | 0.24                | 0.42       |
| (1,503) | 1:625:A:MET:HG2 | 1:629:A:VAL:HG23 | 11                  | 0.47     | 0.24                | 0.42       |
| (1,483) | 1:667:A:LYS:HA  | 1:667:A:LYS:HG3  | 11                  | 0.45     | 0.04                | 0.45       |
| (1,364) | 1:648:A:GLU:HA  | 1:651:A:HIS:HB2  | 11                  | 0.42     | 0.27                | 0.31       |
| (3,5)   | 1:612:A:PHE:HB2 | 2:545:B:LEU:HD21 | 11                  | 0.41     | 0.27                | 0.37       |
| (3,5)   | 1:612:A:PHE:HB2 | 2:545:B:LEU:HD22 | 11                  | 0.41     | 0.27                | 0.37       |
| (3,5)   | 1:612:A:PHE:HB2 | 2:545:B:LEU:HD23 | 11                  | 0.41     | 0.27                | 0.37       |
| (3,5)   | 1:612:A:PHE:HB3 | 2:545:B:LEU:HD21 | 11                  | 0.41     | 0.27                | 0.37       |
| (3,5)   | 1:612:A:PHE:HB3 | 2:545:B:LEU:HD22 | 11                  | 0.41     | 0.27                | 0.37       |
| (3,5)   | 1:612:A:PHE:HB3 | 2:545:B:LEU:HD23 | 11                  | 0.41     | 0.27                | 0.37       |
| (1,447) | 1:599:A:LEU:HB3 | 1:599:A:LEU:HD12 | 11                  | 0.4      | 0.04                | 0.41       |
| (1,447) | 1:599:A:LEU:HB3 | 1:599:A:LEU:HD13 | 11                  | 0.4      | 0.04                | 0.41       |
| (1,447) | 1:599:A:LEU:HB3 | 1:599:A:LEU:HD11 | 11                  | 0.4      | 0.04                | 0.41       |
| (1,677) | 1:643:A:ALA:H   | 1:642:A:SER:HB2  | 11                  | 0.19     | 0.07                | 0.17       |
| (2,244) | 2:535:B:SER:H   | 2:534:B:PHE:HA   | 11                  | 0.12     | 0.02                | 0.11       |
| (1,229) | 1:636:A:GLU:HG2 | 1:604:A:VAL:HG23 | 10                  | 1.41     | 0.63                | 1.44       |
| (1,229) | 1:636:A:GLU:HG2 | 1:604:A:VAL:HG22 | 10                  | 1.41     | 0.63                | 1.44       |
| (1,229) | 1:636:A:GLU:HG2 | 1:604:A:VAL:HG21 | 10                  | 1.41     | 0.63                | 1.44       |
| (1,258) | 1:656:A:LYS:HA  | 1:659:A:LYS:HB3  | 10                  | 1.03     | 0.29                | 1.14       |
| (2,111) | 2:534:B:PHE:HE1 | 2:537:B:ILE:HD11 | 10                  | 0.81     | 0.45                | 0.9        |
| (2,111) | 2:534:B:PHE:HE1 | 2:537:B:ILE:HD12 | 10                  | 0.81     | 0.45                | 0.9        |
| (2,111) | 2:534:B:PHE:HE1 | 2:537:B:ILE:HD13 | 10                  | 0.81     | 0.45                | 0.9        |
| (2,111) | 2:534:B:PHE:HE2 | 2:537:B:ILE:HD11 | 10                  | 0.81     | 0.45                | 0.9        |
| (2,111) | 2:534:B:PHE:HE2 | 2:537:B:ILE:HD12 | 10                  | 0.81     | 0.45                | 0.9        |
| (2,111) | 2:534:B:PHE:HE2 | 2:537:B:ILE:HD13 | 10                  | 0.81     | 0.45                | 0.9        |
| (1,475) | 1:599:A:LEU:HB2 | 1:595:A:VAL:HG11 | 10                  | 0.43     | 0.24                | 0.28       |
| (1,475) | 1:599:A:LEU:HB2 | 1:595:A:VAL:HG13 | 10                  | 0.43     | 0.24                | 0.28       |
| (1,475) | 1:599:A:LEU:HB2 | 1:595:A:VAL:HG12 | 10                  | 0.43     | 0.24                | 0.28       |
| (1,93)  | 1:662:A:LYS:HG3 | 1:662:A:LYS:HE2  | 10                  | 0.39     | 0.22                | 0.24       |
| (1,921) | 1:659:A:LYS:H   | 1:659:A:LYS:HG3  | 10                  | 0.38     | 0.07                | 0.42       |
| (1,592) | 1:634:A:LYS:HG2 | 1:634:A:LYS:HE2  | 10                  | 0.38     | 0.22                | 0.3        |
| (3,10)  | 1:624:A:ARG:HB2 | 2:545:B:LEU:HD11 | 10                  | 0.31     | 0.24                | 0.2        |
| (3,10)  | 1:624:A:ARG:HB2 | 2:545:B:LEU:HD12 | 10                  | 0.31     | 0.24                | 0.2        |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD13 | 10                  | 0.31     | 0.24                | 0.2        |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD11 | 10                  | 0.31     | 0.24                | 0.2        |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD12 | 10                  | 0.31     | 0.24                | 0.2        |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD13 | 10                  | 0.31     | 0.24                | 0.2        |
| (2,127) | 2:542:B:PHE:HA   | 2:545:B:LEU:HB3  | 10                  | 0.21     | 0.07                | 0.2        |
| (1,778) | 1:611:A:ILE:H    | 1:611:A:ILE:HG12 | 10                  | 0.2      | 0.1                 | 0.18       |
| (1,672) | 1:593:A:GLU:H    | 1:593:A:GLU:HG2  | 10                  | 0.19     | 0.06                | 0.16       |
| (2,32)  | 2:549:B:ILE:HA   | 2:549:B:ILE:HG12 | 10                  | 0.16     | 0.02                | 0.16       |
| (2,34)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HA   | 10                  | 0.16     | 0.02                | 0.16       |
| (1,333) | 1:657:A:ILE:HA   | 1:657:A:ILE:HG21 | 10                  | 0.13     | 0.02                | 0.13       |
| (1,333) | 1:657:A:ILE:HA   | 1:657:A:ILE:HG22 | 10                  | 0.13     | 0.02                | 0.13       |
| (1,333) | 1:657:A:ILE:HA   | 1:657:A:ILE:HG23 | 10                  | 0.13     | 0.02                | 0.13       |
| (1,245) | 1:659:A:LYS:HB3  | 1:659:A:LYS:HA   | 10                  | 0.11     | 0.01                | 0.11       |
| (2,203) | 2:535:B:SER:H    | 2:535:B:SER:HB2  | 10                  | 0.11     | 0.01                | 0.11       |
| (1,724) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HD2  | 9                   | 1.76     | 2.17                | 0.51       |
| (1,725) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HG3  | 9                   | 1.75     | 2.41                | 0.7        |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD1  | 9                   | 1.47     | 0.69                | 1.85       |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD2  | 9                   | 1.47     | 0.69                | 1.85       |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD1  | 9                   | 1.47     | 0.69                | 1.85       |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD2  | 9                   | 1.47     | 0.69                | 1.85       |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD1  | 9                   | 1.47     | 0.69                | 1.85       |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD2  | 9                   | 1.47     | 0.69                | 1.85       |
| (1,435) | 1:653:A:LEU:HD11 | 1:639:A:MET:HE1  | 9                   | 1.29     | 0.93                | 0.99       |
| (1,435) | 1:653:A:LEU:HD11 | 1:639:A:MET:HE3  | 9                   | 1.29     | 0.93                | 0.99       |
| (1,435) | 1:653:A:LEU:HD13 | 1:639:A:MET:HE1  | 9                   | 1.29     | 0.93                | 0.99       |
| (1,435) | 1:653:A:LEU:HD12 | 1:639:A:MET:HE2  | 9                   | 1.29     | 0.93                | 0.99       |
| (1,435) | 1:653:A:LEU:HD13 | 1:639:A:MET:HE2  | 9                   | 1.29     | 0.93                | 0.99       |
| (1,435) | 1:653:A:LEU:HD12 | 1:639:A:MET:HE3  | 9                   | 1.29     | 0.93                | 0.99       |
| (1,435) | 1:653:A:LEU:HD11 | 1:639:A:MET:HE2  | 9                   | 1.29     | 0.93                | 0.99       |
| (2,95)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HB3  | 9                   | 0.79     | 0.24                | 0.79       |
| (1,268) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HB3  | 9                   | 0.76     | 0.29                | 0.92       |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD1  | 9                   | 0.73     | 0.33                | 0.69       |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD2  | 9                   | 0.73     | 0.33                | 0.69       |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD1  | 9                   | 0.73     | 0.33                | 0.69       |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD2  | 9                   | 0.73     | 0.33                | 0.69       |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD1  | 9                   | 0.73     | 0.33                | 0.69       |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD2  | 9                   | 0.73     | 0.33                | 0.69       |
| (1,589) | 1:599:A:LEU:HD23 | 1:599:A:LEU:HB2  | 9                   | 0.66     | 0.03                | 0.67       |
| (1,589) | 1:599:A:LEU:HD22 | 1:599:A:LEU:HB2  | 9                   | 0.66     | 0.03                | 0.67       |
| (1,589) | 1:599:A:LEU:HD21 | 1:599:A:LEU:HB2  | 9                   | 0.66     | 0.03                | 0.67       |
| (1,701) | 1:614:A:THR:H    | 1:614:A:THR:HG22 | 9                   | 0.64     | 0.14                | 0.68       |
| (1,701) | 1:614:A:THR:H    | 1:614:A:THR:HG21 | 9                   | 0.64     | 0.14                | 0.68       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,701) | 1:614:A:THR:H    | 1:614:A:THR:HG23 | 9                   | 0.64     | 0.14                | 0.68       |
| (1,212) | 1:611:A:ILE:HD11 | 1:607:A:LEU:HD23 | 9                   | 0.63     | 0.19                | 0.64       |
| (1,212) | 1:611:A:ILE:HD12 | 1:607:A:LEU:HD23 | 9                   | 0.63     | 0.19                | 0.64       |
| (1,212) | 1:611:A:ILE:HD13 | 1:607:A:LEU:HD23 | 9                   | 0.63     | 0.19                | 0.64       |
| (1,212) | 1:611:A:ILE:HD11 | 1:607:A:LEU:HD22 | 9                   | 0.63     | 0.19                | 0.64       |
| (1,212) | 1:611:A:ILE:HD12 | 1:607:A:LEU:HD22 | 9                   | 0.63     | 0.19                | 0.64       |
| (1,212) | 1:611:A:ILE:HD13 | 1:607:A:LEU:HD22 | 9                   | 0.63     | 0.19                | 0.64       |
| (1,212) | 1:611:A:ILE:HD11 | 1:607:A:LEU:HD21 | 9                   | 0.63     | 0.19                | 0.64       |
| (1,212) | 1:611:A:ILE:HD12 | 1:607:A:LEU:HD21 | 9                   | 0.63     | 0.19                | 0.64       |
| (1,212) | 1:611:A:ILE:HD13 | 1:607:A:LEU:HD21 | 9                   | 0.63     | 0.19                | 0.64       |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 9                   | 0.59     | 0.49                | 0.35       |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 9                   | 0.59     | 0.49                | 0.35       |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 9                   | 0.59     | 0.49                | 0.35       |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 9                   | 0.59     | 0.49                | 0.35       |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 9                   | 0.59     | 0.49                | 0.35       |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 9                   | 0.59     | 0.49                | 0.35       |
| (1,172) | 1:651:A:HIS:HB2  | 1:651:A:HIS:HD2  | 9                   | 0.52     | 0.08                | 0.46       |
| (1,580) | 1:599:A:LEU:HD13 | 1:599:A:LEU:HA   | 9                   | 0.46     | 0.19                | 0.59       |
| (1,580) | 1:599:A:LEU:HD11 | 1:599:A:LEU:HA   | 9                   | 0.46     | 0.19                | 0.59       |
| (1,580) | 1:599:A:LEU:HD12 | 1:599:A:LEU:HA   | 9                   | 0.46     | 0.19                | 0.59       |
| (1,783) | 1:616:A:ASP:H    | 1:615:A:PRO:HD3  | 9                   | 0.35     | 0.05                | 0.37       |
| (1,590) | 1:599:A:LEU:HG   | 1:599:A:LEU:HB3  | 9                   | 0.35     | 0.02                | 0.36       |
| (1,122) | 1:595:A:VAL:HG23 | 1:649:A:TYR:HE1  | 9                   | 0.28     | 0.17                | 0.26       |
| (1,122) | 1:595:A:VAL:HG23 | 1:649:A:TYR:HE2  | 9                   | 0.28     | 0.17                | 0.26       |
| (1,122) | 1:595:A:VAL:HG21 | 1:649:A:TYR:HE1  | 9                   | 0.28     | 0.17                | 0.26       |
| (1,122) | 1:595:A:VAL:HG21 | 1:649:A:TYR:HE2  | 9                   | 0.28     | 0.17                | 0.26       |
| (1,122) | 1:595:A:VAL:HG22 | 1:649:A:TYR:HE1  | 9                   | 0.28     | 0.17                | 0.26       |
| (1,122) | 1:595:A:VAL:HG22 | 1:649:A:TYR:HE2  | 9                   | 0.28     | 0.17                | 0.26       |
| (1,732) | 1:594:A:HIS:H    | 1:593:A:GLU:HB3  | 9                   | 0.23     | 0.09                | 0.23       |
| (2,76)  | 2:542:B:PHE:HA   | 2:542:B:PHE:HD1  | 9                   | 0.2      | 0.14                | 0.16       |
| (2,76)  | 2:542:B:PHE:HA   | 2:542:B:PHE:HD2  | 9                   | 0.2      | 0.14                | 0.16       |
| (1,359) | 1:603:A:LEU:HD13 | 1:599:A:LEU:HD21 | 8                   | 1.77     | 0.77                | 1.84       |
| (1,359) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD23 | 8                   | 1.77     | 0.77                | 1.84       |
| (1,359) | 1:603:A:LEU:HD11 | 1:599:A:LEU:HD22 | 8                   | 1.77     | 0.77                | 1.84       |
| (1,359) | 1:603:A:LEU:HD11 | 1:599:A:LEU:HD23 | 8                   | 1.77     | 0.77                | 1.84       |
| (1,359) | 1:603:A:LEU:HD11 | 1:599:A:LEU:HD21 | 8                   | 1.77     | 0.77                | 1.84       |
| (1,359) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD21 | 8                   | 1.77     | 0.77                | 1.84       |
| (1,208) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD12 | 8                   | 1.63     | 0.08                | 1.62       |
| (1,208) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD13 | 8                   | 1.63     | 0.08                | 1.62       |
| (1,208) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD11 | 8                   | 1.63     | 0.08                | 1.62       |
| (1,793) | 1:618:A:ALA:H    | 1:617:A:PRO:HG2  | 8                   | 1.28     | 0.05                | 1.3        |
| (2,169) | 2:544:B:ALA:HA   | 2:547:B:SER:HB3  | 8                   | 0.47     | 0.23                | 0.47       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,38)   | 1:609:A:GLN:HB2  | 1:609:A:GLN:HG2  | 8                   | 0.45     | 0.0                 | 0.45       |
| (1,606)  | 1:595:A:VAL:HA   | 1:599:A:LEU:HD21 | 8                   | 0.45     | 0.2                 | 0.44       |
| (1,606)  | 1:595:A:VAL:HA   | 1:599:A:LEU:HD23 | 8                   | 0.45     | 0.2                 | 0.44       |
| (1,606)  | 1:595:A:VAL:HA   | 1:599:A:LEU:HD22 | 8                   | 0.45     | 0.2                 | 0.44       |
| (1,221)  | 1:607:A:LEU:HB3  | 1:604:A:VAL:HA   | 8                   | 0.4      | 0.13                | 0.44       |
| (1,97)   | 1:662:A:LYS:HB2  | 1:662:A:LYS:HD3  | 8                   | 0.39     | 0.29                | 0.2        |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD1  | 8                   | 0.33     | 0.11                | 0.32       |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD2  | 8                   | 0.33     | 0.11                | 0.32       |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD1  | 8                   | 0.33     | 0.11                | 0.32       |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD2  | 8                   | 0.33     | 0.11                | 0.32       |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD1  | 8                   | 0.33     | 0.11                | 0.32       |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD2  | 8                   | 0.33     | 0.11                | 0.32       |
| (1,845)  | 1:632:A:ALA:H    | 1:631:A:TYR:HD1  | 8                   | 0.3      | 0.12                | 0.31       |
| (1,845)  | 1:632:A:ALA:H    | 1:631:A:TYR:HD2  | 8                   | 0.3      | 0.12                | 0.31       |
| (1,459)  | 1:607:A:LEU:HB2  | 1:607:A:LEU:HD21 | 8                   | 0.27     | 0.1                 | 0.28       |
| (1,459)  | 1:607:A:LEU:HB2  | 1:607:A:LEU:HD22 | 8                   | 0.27     | 0.1                 | 0.28       |
| (1,459)  | 1:607:A:LEU:HB2  | 1:607:A:LEU:HD23 | 8                   | 0.27     | 0.1                 | 0.28       |
| (1,91)   | 1:662:A:LYS:HG2  | 1:662:A:LYS:HE2  | 8                   | 0.2      | 0.05                | 0.23       |
| (2,144)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD21 | 8                   | 0.2      | 0.05                | 0.22       |
| (2,144)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD22 | 8                   | 0.2      | 0.05                | 0.22       |
| (2,144)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD23 | 8                   | 0.2      | 0.05                | 0.22       |
| (1,300)  | 1:617:A:PRO:HA   | 1:617:A:PRO:HB2  | 8                   | 0.13     | 0.0                 | 0.13       |
| (3,21)   | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD1  | 7                   | 0.84     | 0.61                | 1.0        |
| (3,21)   | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD2  | 7                   | 0.84     | 0.61                | 1.0        |
| (3,21)   | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD1  | 7                   | 0.84     | 0.61                | 1.0        |
| (3,21)   | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD2  | 7                   | 0.84     | 0.61                | 1.0        |
| (3,21)   | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD1  | 7                   | 0.84     | 0.61                | 1.0        |
| (3,21)   | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD2  | 7                   | 0.84     | 0.61                | 1.0        |
| (1,944)  | 1:666:A:GLU:H    | 1:666:A:GLU:HG2  | 7                   | 0.74     | 0.46                | 1.11       |
| (1,275)  | 1:593:A:GLU:HB3  | 1:593:A:GLU:HG2  | 7                   | 0.56     | 0.07                | 0.59       |
| (2,267)  | 2:542:B:PHE:H    | 2:540:B:MET:HB2  | 7                   | 0.47     | 0.08                | 0.49       |
| (2,72)   | 2:537:B:ILE:HB   | 2:534:B:PHE:HD1  | 7                   | 0.41     | 0.2                 | 0.3        |
| (2,72)   | 2:537:B:ILE:HB   | 2:534:B:PHE:HD2  | 7                   | 0.41     | 0.2                 | 0.3        |
| (1,973)  | 1:655:A:GLU:H    | 1:651:A:HIS:HA   | 7                   | 0.13     | 0.02                | 0.12       |
| (1,991)  | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 6                   | 1.0      | 0.21                | 0.98       |
| (1,992)  | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 6                   | 1.0      | 0.21                | 0.98       |
| (1,415)  | 1:620:A:LEU:HD21 | 1:625:A:MET:HG2  | 6                   | 0.84     | 0.84                | 0.52       |
| (1,415)  | 1:620:A:LEU:HD22 | 1:625:A:MET:HG2  | 6                   | 0.84     | 0.84                | 0.52       |
| (1,384)  | 1:614:A:THR:HG22 | 1:614:A:THR:HA   | 6                   | 0.65     | 0.03                | 0.64       |
| (1,384)  | 1:614:A:THR:HG23 | 1:614:A:THR:HA   | 6                   | 0.65     | 0.03                | 0.64       |
| (1,384)  | 1:614:A:THR:HG21 | 1:614:A:THR:HA   | 6                   | 0.65     | 0.03                | 0.64       |
| (1,118)  | 1:653:A:LEU:HB3  | 1:650:A:TYR:HA   | 6                   | 0.6      | 0.37                | 0.52       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG11 | 6                   | 0.57     | 0.32                | 0.62       |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG12 | 6                   | 0.57     | 0.32                | 0.62       |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG13 | 6                   | 0.57     | 0.32                | 0.62       |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG11 | 6                   | 0.57     | 0.32                | 0.62       |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG12 | 6                   | 0.57     | 0.32                | 0.62       |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG13 | 6                   | 0.57     | 0.32                | 0.62       |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG11 | 6                   | 0.57     | 0.32                | 0.62       |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG12 | 6                   | 0.57     | 0.32                | 0.62       |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG13 | 6                   | 0.57     | 0.32                | 0.62       |
| (1,935)  | 1:663:A:GLU:H    | 1:663:A:GLU:HG2  | 6                   | 0.55     | 0.06                | 0.55       |
| (1,95)   | 1:662:A:LYS:HD2  | 1:662:A:LYS:HE2  | 6                   | 0.55     | 0.01                | 0.54       |
| (1,96)   | 1:662:A:LYS:HG2  | 1:662:A:LYS:HD3  | 6                   | 0.48     | 0.01                | 0.48       |
| (1,3)    | 1:639:A:MET:HG3  | 1:639:A:MET:HE2  | 6                   | 0.41     | 0.2                 | 0.49       |
| (1,3)    | 1:639:A:MET:HG3  | 1:639:A:MET:HE3  | 6                   | 0.41     | 0.2                 | 0.49       |
| (1,3)    | 1:639:A:MET:HG3  | 1:639:A:MET:HE1  | 6                   | 0.41     | 0.2                 | 0.49       |
| (3,25)   | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG21 | 6                   | 0.33     | 0.06                | 0.31       |
| (3,25)   | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG22 | 6                   | 0.33     | 0.06                | 0.31       |
| (3,25)   | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG23 | 6                   | 0.33     | 0.06                | 0.31       |
| (3,25)   | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG21 | 6                   | 0.33     | 0.06                | 0.31       |
| (3,25)   | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG22 | 6                   | 0.33     | 0.06                | 0.31       |
| (3,25)   | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG23 | 6                   | 0.33     | 0.06                | 0.31       |
| (1,695)  | 1:641:A:GLU:H    | 1:641:A:GLU:HG2  | 6                   | 0.32     | 0.35                | 0.18       |
| (1,94)   | 1:662:A:LYS:HD3  | 1:662:A:LYS:HE3  | 6                   | 0.3      | 0.01                | 0.3        |
| (1,272)  | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB2  | 6                   | 0.18     | 0.03                | 0.2        |
| (1,90)   | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE3  | 6                   | 0.16     | 0.02                | 0.16       |
| (1,455)  | 1:614:A:THR:HB   | 1:614:A:THR:HA   | 6                   | 0.15     | 0.0                 | 0.15       |
| (1,337)  | 1:611:A:ILE:HD13 | 1:611:A:ILE:HB   | 6                   | 0.15     | 0.06                | 0.13       |
| (1,337)  | 1:611:A:ILE:HD11 | 1:611:A:ILE:HB   | 6                   | 0.15     | 0.06                | 0.13       |
| (1,337)  | 1:611:A:ILE:HD12 | 1:611:A:ILE:HB   | 6                   | 0.15     | 0.06                | 0.13       |
| (1,982)  | 1:607:A:LEU:H    | 1:606:A:LYS:HB2  | 6                   | 0.15     | 0.04                | 0.15       |
| (1,155)  | 1:605:A:HIS:HB2  | 1:602:A:HIS:HA   | 6                   | 0.15     | 0.02                | 0.14       |
| (1,689)  | 1:670:A:SER:H    | 1:670:A:SER:HB2  | 6                   | 0.12     | 0.02                | 0.12       |
| (1,573)  | 1:657:A:ILE:HD12 | 1:606:A:LYS:HG2  | 5                   | 1.68     | 0.26                | 1.8        |
| (1,573)  | 1:657:A:ILE:HD11 | 1:606:A:LYS:HG2  | 5                   | 1.68     | 0.26                | 1.8        |
| (1,573)  | 1:657:A:ILE:HD13 | 1:606:A:LYS:HG2  | 5                   | 1.68     | 0.26                | 1.8        |
| (1,263)  | 1:607:A:LEU:HD21 | 1:632:A:ALA:HB1  | 5                   | 1.28     | 0.46                | 1.34       |
| (1,263)  | 1:607:A:LEU:HD22 | 1:632:A:ALA:HB1  | 5                   | 1.28     | 0.46                | 1.34       |
| (1,263)  | 1:607:A:LEU:HD21 | 1:632:A:ALA:HB2  | 5                   | 1.28     | 0.46                | 1.34       |
| (1,263)  | 1:607:A:LEU:HD22 | 1:632:A:ALA:HB2  | 5                   | 1.28     | 0.46                | 1.34       |
| (1,32)   | 1:648:A:GLU:HB2  | 1:643:A:ALA:HB2  | 5                   | 1.17     | 0.09                | 1.13       |
| (1,32)   | 1:648:A:GLU:HB2  | 1:643:A:ALA:HB1  | 5                   | 1.17     | 0.09                | 1.13       |
| (1,32)   | 1:648:A:GLU:HB2  | 1:643:A:ALA:HB3  | 5                   | 1.17     | 0.09                | 1.13       |

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| Key     | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,656) | 1:623:A:ARG:HG2 | 1:623:A:ARG:HA   | 5                   | 0.78     | 0.02                | 0.79       |
| (1,875) | 1:645:A:SER:H   | 1:648:A:GLU:HB2  | 5                   | 0.72     | 0.09                | 0.7        |
| (2,69)  | 2:534:B:PHE:HA  | 2:534:B:PHE:HD1  | 5                   | 0.61     | 0.21                | 0.6        |
| (2,69)  | 2:534:B:PHE:HA  | 2:534:B:PHE:HD2  | 5                   | 0.61     | 0.21                | 0.6        |
| (2,260) | 2:540:B:MET:H   | 2:540:B:MET:HG3  | 5                   | 0.59     | 0.01                | 0.59       |
| (3,13)  | 1:625:A:MET:HA  | 2:545:B:LEU:HD21 | 5                   | 0.59     | 0.3                 | 0.63       |
| (3,13)  | 1:625:A:MET:HA  | 2:545:B:LEU:HD22 | 5                   | 0.59     | 0.3                 | 0.63       |
| (3,13)  | 1:625:A:MET:HA  | 2:545:B:LEU:HD23 | 5                   | 0.59     | 0.3                 | 0.63       |
| (2,132) | 2:546:B:LEU:HB2 | 2:543:B:SER:HA   | 5                   | 0.49     | 0.06                | 0.53       |
| (1,186) | 1:621:A:LYS:HA  | 1:621:A:LYS:HG3  | 5                   | 0.36     | 0.03                | 0.36       |
| (1,950) | 1:671:A:ARG:H   | 1:671:A:ARG:HB2  | 5                   | 0.32     | 0.06                | 0.34       |
| (2,137) | 2:543:B:SER:HA  | 2:546:B:LEU:HB2  | 5                   | 0.31     | 0.21                | 0.25       |
| (1,355) | 1:593:A:GLU:HA  | 1:593:A:GLU:HG2  | 5                   | 0.28     | 0.13                | 0.32       |
| (1,23)  | 1:653:A:LEU:HB3 | 1:653:A:LEU:HD11 | 5                   | 0.21     | 0.07                | 0.2        |
| (1,23)  | 1:653:A:LEU:HB3 | 1:653:A:LEU:HD12 | 5                   | 0.21     | 0.07                | 0.2        |
| (1,399) | 1:607:A:LEU:HA  | 1:610:A:ALA:HB1  | 5                   | 0.17     | 0.02                | 0.17       |
| (1,399) | 1:607:A:LEU:HA  | 1:610:A:ALA:HB3  | 5                   | 0.17     | 0.02                | 0.17       |
| (1,696) | 1:614:A:THR:H   | 1:614:A:THR:HB   | 5                   | 0.17     | 0.01                | 0.17       |
| (2,181) | 2:540:B:MET:HA  | 2:540:B:MET:HB2  | 5                   | 0.14     | 0.01                | 0.14       |
| (1,764) | 1:606:A:LYS:H   | 1:602:A:HIS:HA   | 5                   | 0.14     | 0.01                | 0.14       |
| (1,526) | 1:646:A:ARG:HG2 | 1:646:A:ARG:HD3  | 5                   | 0.1      | 0.0                 | 0.1        |
| (1,185) | 1:621:A:LYS:HD2 | 1:621:A:LYS:HB2  | 4                   | 0.94     | 0.01                | 0.94       |
| (1,210) | 1:632:A:ALA:HA  | 1:607:A:LEU:HD22 | 4                   | 0.68     | 0.33                | 0.6        |
| (1,210) | 1:632:A:ALA:HA  | 1:607:A:LEU:HD21 | 4                   | 0.68     | 0.33                | 0.6        |
| (1,450) | 1:665:A:GLU:HA  | 1:665:A:GLU:HG2  | 4                   | 0.61     | 0.31                | 0.5        |
| (1,540) | 1:653:A:LEU:HA  | 1:653:A:LEU:HD13 | 4                   | 0.4      | 0.27                | 0.38       |
| (1,540) | 1:653:A:LEU:HA  | 1:653:A:LEU:HD11 | 4                   | 0.4      | 0.27                | 0.38       |
| (2,250) | 2:534:B:PHE:H   | 2:534:B:PHE:HD1  | 4                   | 0.36     | 0.22                | 0.28       |
| (1,665) | 1:592:A:HIS:H   | 1:592:A:HIS:HB2  | 4                   | 0.3      | 0.05                | 0.3        |
| (2,77)  | 2:547:B:SER:HB3 | 2:544:B:ALA:HA   | 4                   | 0.27     | 0.1                 | 0.26       |
| (1,805) | 1:621:A:LYS:H   | 1:621:A:LYS:HG3  | 4                   | 0.23     | 0.04                | 0.24       |
| (3,18)  | 1:627:A:ASN:HB2 | 2:537:B:ILE:HG21 | 4                   | 0.17     | 0.06                | 0.17       |
| (3,18)  | 1:627:A:ASN:HB2 | 2:537:B:ILE:HG22 | 4                   | 0.17     | 0.06                | 0.17       |
| (3,18)  | 1:627:A:ASN:HB2 | 2:537:B:ILE:HG23 | 4                   | 0.17     | 0.06                | 0.17       |
| (1,949) | 1:671:A:ARG:H   | 1:671:A:ARG:HB3  | 4                   | 0.17     | 0.0                 | 0.17       |
| (2,256) | 2:538:B:ALA:H   | 2:537:B:ILE:HG22 | 4                   | 0.17     | 0.04                | 0.17       |
| (2,256) | 2:538:B:ALA:H   | 2:537:B:ILE:HG21 | 4                   | 0.17     | 0.04                | 0.17       |
| (1,173) | 1:651:A:HIS:HA  | 1:651:A:HIS:HB2  | 4                   | 0.15     | 0.02                | 0.14       |
| (2,264) | 2:541:B:ASP:H   | 2:540:B:MET:HB3  | 4                   | 0.14     | 0.02                | 0.14       |
| (1,444) | 1:625:A:MET:HG3 | 1:625:A:MET:HE1  | 4                   | 0.13     | 0.01                | 0.13       |
| (1,444) | 1:625:A:MET:HG3 | 1:625:A:MET:HE3  | 4                   | 0.13     | 0.01                | 0.13       |
| (1,444) | 1:625:A:MET:HG3 | 1:625:A:MET:HE2  | 4                   | 0.13     | 0.01                | 0.13       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,184)  | 2:540:B:MET:HG3  | 2:540:B:MET:HB2  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,262)  | 1:629:A:VAL:HA   | 1:632:A:ALA:HB1  | 4                   | 0.11     | 0.02                | 0.11       |
| (1,262)  | 1:629:A:VAL:HA   | 1:632:A:ALA:HB3  | 4                   | 0.11     | 0.02                | 0.11       |
| (1,1007) | 1:640:A:TYR:HA   | 1:591:A:TRP:HZ2  | 3                   | 2.5      | 3.29                | 0.18       |
| (3,7)    | 1:612:A:PHE:HE1  | 2:546:B:LEU:HD21 | 3                   | 2.31     | 1.28                | 1.42       |
| (3,7)    | 1:612:A:PHE:HE1  | 2:546:B:LEU:HD22 | 3                   | 2.31     | 1.28                | 1.42       |
| (3,7)    | 1:612:A:PHE:HE1  | 2:546:B:LEU:HD23 | 3                   | 2.31     | 1.28                | 1.42       |
| (3,7)    | 1:612:A:PHE:HE2  | 2:546:B:LEU:HD21 | 3                   | 2.31     | 1.28                | 1.42       |
| (3,7)    | 1:612:A:PHE:HE2  | 2:546:B:LEU:HD22 | 3                   | 2.31     | 1.28                | 1.42       |
| (3,7)    | 1:612:A:PHE:HE2  | 2:546:B:LEU:HD23 | 3                   | 2.31     | 1.28                | 1.42       |
| (1,375)  | 1:633:A:LYS:HD2  | 1:629:A:VAL:HG13 | 3                   | 1.11     | 1.22                | 0.37       |
| (1,456)  | 1:608:A:VAL:HB   | 1:605:A:HIS:HA   | 3                   | 1.02     | 0.55                | 1.31       |
| (1,380)  | 1:620:A:LEU:HD12 | 1:617:A:PRO:HA   | 3                   | 0.9      | 0.76                | 0.59       |
| (1,380)  | 1:620:A:LEU:HD13 | 1:617:A:PRO:HA   | 3                   | 0.9      | 0.76                | 0.59       |
| (1,721)  | 1:609:A:GLN:H    | 1:608:A:VAL:HB   | 3                   | 0.78     | 0.02                | 0.78       |
| (1,465)  | 1:589:A:LYS:HG2  | 1:589:A:LYS:HE2  | 3                   | 0.61     | 0.04                | 0.58       |
| (3,12)   | 1:625:A:MET:HA   | 2:545:B:LEU:HD11 | 3                   | 0.51     | 0.16                | 0.49       |
| (3,12)   | 1:625:A:MET:HA   | 2:545:B:LEU:HD12 | 3                   | 0.51     | 0.16                | 0.49       |
| (3,12)   | 1:625:A:MET:HA   | 2:545:B:LEU:HD13 | 3                   | 0.51     | 0.16                | 0.49       |
| (1,84)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HG2  | 3                   | 0.5      | 0.02                | 0.51       |
| (1,469)  | 1:635:A:VAL:HA   | 1:635:A:VAL:HG13 | 3                   | 0.44     | 0.22                | 0.49       |
| (1,469)  | 1:635:A:VAL:HA   | 1:635:A:VAL:HG11 | 3                   | 0.44     | 0.22                | 0.49       |
| (1,284)  | 1:671:A:ARG:HG2  | 1:671:A:ARG:HA   | 3                   | 0.41     | 0.03                | 0.4        |
| (1,162)  | 1:594:A:HIS:HB2  | 1:594:A:HIS:HD2  | 3                   | 0.37     | 0.03                | 0.36       |
| (3,32)   | 1:664:A:LEU:HD11 | 2:542:B:PHE:HE1  | 3                   | 0.35     | 0.24                | 0.23       |
| (3,32)   | 1:664:A:LEU:HD11 | 2:542:B:PHE:HE2  | 3                   | 0.35     | 0.24                | 0.23       |
| (3,32)   | 1:664:A:LEU:HD12 | 2:542:B:PHE:HE1  | 3                   | 0.35     | 0.24                | 0.23       |
| (3,32)   | 1:664:A:LEU:HD12 | 2:542:B:PHE:HE2  | 3                   | 0.35     | 0.24                | 0.23       |
| (3,32)   | 1:664:A:LEU:HD13 | 2:542:B:PHE:HE1  | 3                   | 0.35     | 0.24                | 0.23       |
| (3,32)   | 1:664:A:LEU:HD13 | 2:542:B:PHE:HE2  | 3                   | 0.35     | 0.24                | 0.23       |
| (3,31)   | 1:664:A:LEU:HD11 | 2:542:B:PHE:HD1  | 3                   | 0.31     | 0.09                | 0.32       |
| (3,31)   | 1:664:A:LEU:HD11 | 2:542:B:PHE:HD2  | 3                   | 0.31     | 0.09                | 0.32       |
| (3,31)   | 1:664:A:LEU:HD12 | 2:542:B:PHE:HD1  | 3                   | 0.31     | 0.09                | 0.32       |
| (3,31)   | 1:664:A:LEU:HD12 | 2:542:B:PHE:HD2  | 3                   | 0.31     | 0.09                | 0.32       |
| (3,31)   | 1:664:A:LEU:HD13 | 2:542:B:PHE:HD1  | 3                   | 0.31     | 0.09                | 0.32       |
| (3,31)   | 1:664:A:LEU:HD13 | 2:542:B:PHE:HD2  | 3                   | 0.31     | 0.09                | 0.32       |
| (1,631)  | 1:645:A:SER:HA   | 1:645:A:SER:HB2  | 3                   | 0.27     | 0.0                 | 0.27       |
| (1,549)  | 1:603:A:LEU:HD23 | 1:606:A:LYS:HD2  | 3                   | 0.22     | 0.05                | 0.2        |
| (1,549)  | 1:603:A:LEU:HD22 | 1:606:A:LYS:HD2  | 3                   | 0.22     | 0.05                | 0.2        |
| (2,185)  | 2:540:B:MET:HG3  | 2:540:B:MET:HB3  | 3                   | 0.22     | 0.02                | 0.23       |
| (1,574)  | 1:657:A:ILE:HD13 | 1:657:A:ILE:HG22 | 3                   | 0.14     | 0.02                | 0.14       |
| (1,574)  | 1:657:A:ILE:HD13 | 1:657:A:ILE:HG21 | 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) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,574) | 1:657:A:ILE:HD13 | 1:657:A:ILE:HG23 | 3                   | 0.14     | 0.02                | 0.14       |
| (1,984) | 1:607:A:LEU:H    | 1:607:A:LEU:HB3  | 3                   | 0.14     | 0.02                | 0.14       |
| (1,230) | 1:604:A:VAL:HG21 | 1:604:A:VAL:HA   | 3                   | 0.14     | 0.04                | 0.12       |
| (1,230) | 1:604:A:VAL:HG23 | 1:604:A:VAL:HA   | 3                   | 0.14     | 0.04                | 0.12       |
| (1,140) | 1:643:A:ALA:HB3  | 1:640:A:TYR:HA   | 3                   | 0.13     | 0.03                | 0.12       |
| (1,140) | 1:643:A:ALA:HB2  | 1:640:A:TYR:HA   | 3                   | 0.13     | 0.03                | 0.12       |
| (2,86)  | 2:533:B:ASP:HB2  | 2:533:B:ASP:HA   | 3                   | 0.11     | 0.0                 | 0.11       |
| (2,118) | 2:540:B:MET:HG2  | 2:540:B:MET:HA   | 3                   | 0.11     | 0.01                | 0.1        |
| (2,232) | 2:547:B:SER:H    | 2:546:B:LEU:HA   | 3                   | 0.1      | 0.0                 | 0.1        |
| (3,8)   | 1:612:A:PHE:HE1  | 2:546:B:LEU:HA   | 2                   | 2.4      | 1.94                | 2.4        |
| (3,8)   | 1:612:A:PHE:HE2  | 2:546:B:LEU:HA   | 2                   | 2.4      | 1.94                | 2.4        |
| (1,643) | 1:608:A:VAL:HG21 | 1:608:A:VAL:HA   | 2                   | 1.19     | 0.0                 | 1.19       |
| (1,643) | 1:608:A:VAL:HG23 | 1:608:A:VAL:HA   | 2                   | 1.19     | 0.0                 | 1.19       |
| (3,6)   | 1:612:A:PHE:HE1  | 2:545:B:LEU:HD21 | 2                   | 1.03     | 0.62                | 1.03       |
| (3,6)   | 1:612:A:PHE:HE1  | 2:545:B:LEU:HD22 | 2                   | 1.03     | 0.62                | 1.03       |
| (3,6)   | 1:612:A:PHE:HE1  | 2:545:B:LEU:HD23 | 2                   | 1.03     | 0.62                | 1.03       |
| (3,6)   | 1:612:A:PHE:HE2  | 2:545:B:LEU:HD21 | 2                   | 1.03     | 0.62                | 1.03       |
| (3,6)   | 1:612:A:PHE:HE2  | 2:545:B:LEU:HD22 | 2                   | 1.03     | 0.62                | 1.03       |
| (3,6)   | 1:612:A:PHE:HE2  | 2:545:B:LEU:HD23 | 2                   | 1.03     | 0.62                | 1.03       |
| (2,1)   | 2:542:B:PHE:HA   | 2:545:B:LEU:HD11 | 2                   | 0.9      | 0.55                | 0.9        |
| (2,1)   | 2:542:B:PHE:HA   | 2:545:B:LEU:HD12 | 2                   | 0.9      | 0.55                | 0.9        |
| (2,1)   | 2:542:B:PHE:HA   | 2:545:B:LEU:HD13 | 2                   | 0.9      | 0.55                | 0.9        |
| (1,989) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD21 | 2                   | 0.72     | 0.38                | 0.72       |
| (1,989) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD22 | 2                   | 0.72     | 0.38                | 0.72       |
| (1,989) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD23 | 2                   | 0.72     | 0.38                | 0.72       |
| (1,989) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD21 | 2                   | 0.72     | 0.38                | 0.72       |
| (1,989) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD22 | 2                   | 0.72     | 0.38                | 0.72       |
| (1,989) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD23 | 2                   | 0.72     | 0.38                | 0.72       |
| (1,914) | 1:657:A:ILE:H    | 1:656:A:LYS:HB2  | 2                   | 0.61     | 0.0                 | 0.61       |
| (3,34)  | 1:664:A:LEU:HD21 | 2:542:B:PHE:HE1  | 2                   | 0.45     | 0.09                | 0.45       |
| (3,34)  | 1:664:A:LEU:HD21 | 2:542:B:PHE:HE2  | 2                   | 0.45     | 0.09                | 0.45       |
| (3,34)  | 1:664:A:LEU:HD22 | 2:542:B:PHE:HE1  | 2                   | 0.45     | 0.09                | 0.45       |
| (3,34)  | 1:664:A:LEU:HD22 | 2:542:B:PHE:HE2  | 2                   | 0.45     | 0.09                | 0.45       |
| (3,34)  | 1:664:A:LEU:HD23 | 2:542:B:PHE:HE1  | 2                   | 0.45     | 0.09                | 0.45       |
| (3,34)  | 1:664:A:LEU:HD23 | 2:542:B:PHE:HE2  | 2                   | 0.45     | 0.09                | 0.45       |
| (1,472) | 1:662:A:LYS:HA   | 1:665:A:GLU:HB2  | 2                   | 0.4      | 0.22                | 0.4        |
| (1,125) | 1:603:A:LEU:HD23 | 1:650:A:TYR:HE1  | 2                   | 0.4      | 0.29                | 0.4        |
| (1,125) | 1:603:A:LEU:HD23 | 1:650:A:TYR:HE2  | 2                   | 0.4      | 0.29                | 0.4        |
| (1,125) | 1:603:A:LEU:HD21 | 1:650:A:TYR:HE1  | 2                   | 0.4      | 0.29                | 0.4        |
| (1,125) | 1:603:A:LEU:HD21 | 1:650:A:TYR:HE2  | 2                   | 0.4      | 0.29                | 0.4        |
| (1,808) | 1:622:A:ASP:H    | 1:622:A:ASP:HB3  | 2                   | 0.36     | 0.01                | 0.36       |
| (1,630) | 1:628:A:LEU:HB3  | 1:628:A:LEU:HD11 | 2                   | 0.33     | 0.1                 | 0.33       |

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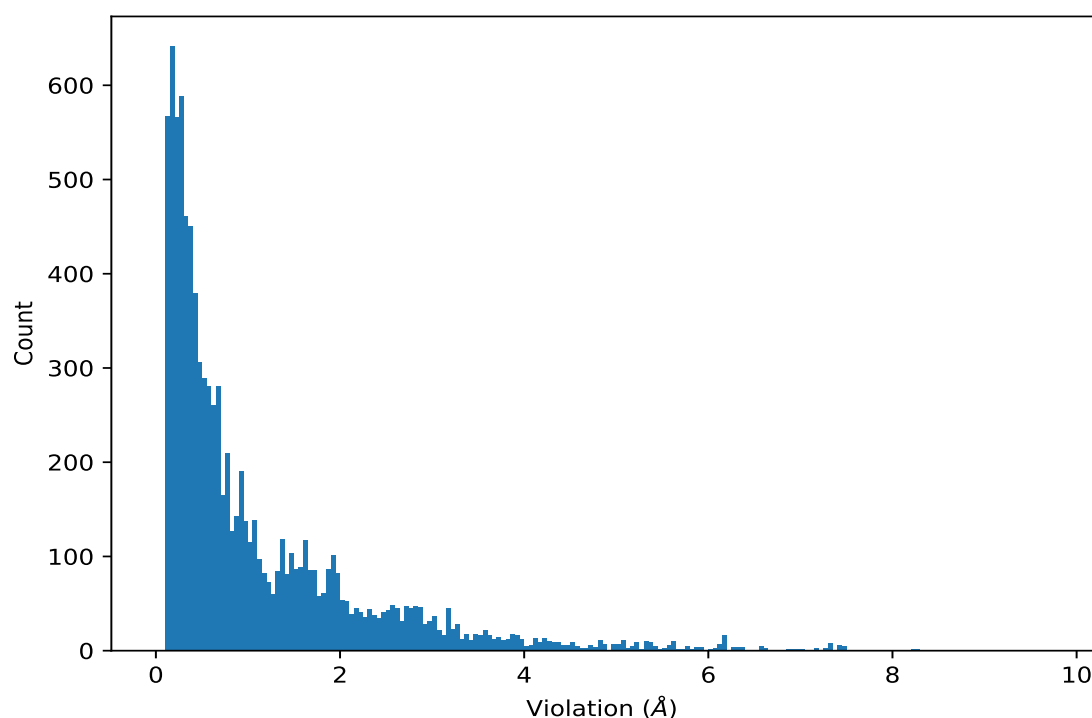
| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,630) | 1:628:A:LEU:HB3  | 1:628:A:LEU:HD13 | 2                   | 0.33     | 0.1                 | 0.33       |
| (2,68)  | 2:545:B:LEU:HA   | 2:545:B:LEU:HD21 | 2                   | 0.33     | 0.01                | 0.33       |
| (2,68)  | 2:545:B:LEU:HA   | 2:545:B:LEU:HD22 | 2                   | 0.33     | 0.01                | 0.33       |
| (2,68)  | 2:545:B:LEU:HA   | 2:545:B:LEU:HD23 | 2                   | 0.33     | 0.01                | 0.33       |
| (1,156) | 1:602:A:HIS:HA   | 1:605:A:HIS:HB3  | 2                   | 0.28     | 0.05                | 0.28       |
| (1,242) | 1:668:A:ARG:HB2  | 1:665:A:GLU:HA   | 2                   | 0.26     | 0.08                | 0.26       |
| (1,443) | 1:625:A:MET:HG2  | 1:625:A:MET:HE1  | 2                   | 0.26     | 0.05                | 0.26       |
| (1,204) | 1:620:A:LEU:HB3  | 1:620:A:LEU:HD22 | 2                   | 0.22     | 0.12                | 0.22       |
| (2,125) | 2:545:B:LEU:HB2  | 2:542:B:PHE:HA   | 2                   | 0.22     | 0.04                | 0.22       |
| (1,101) | 1:658:A:TYR:HB3  | 1:658:A:TYR:HA   | 2                   | 0.21     | 0.0                 | 0.21       |
| (1,77)  | 1:672:A:LEU:HD11 | 1:672:A:LEU:HB3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,77)  | 1:672:A:LEU:HD13 | 1:672:A:LEU:HB3  | 2                   | 0.16     | 0.02                | 0.16       |
| (2,261) | 2:540:B:MET:H    | 2:539:B:ASP:HB2  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,894) | 1:652:A:LEU:H    | 1:652:A:LEU:HD13 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,78)  | 1:672:A:LEU:HB2  | 1:672:A:LEU:HD12 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,537) | 1:653:A:LEU:HD23 | 1:653:A:LEU:HD13 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,89)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HE3  | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2 | 2        | 9.68          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1 | 3        | 8.28          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2 | 3        | 8.28          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1 | 12       | 8.21          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2 | 12       | 8.21          |
| (1,1008) | 1:640:A:TYR:HA   | 1:591:A:TRP:HH2 | 2        | 7.79          |
| (1,7)    | 1:628:A:LEU:HD23 | 1:625:A:MET:HE3 | 18       | 7.62          |
| (1,482)  | 1:664:A:LEU:HD11 | 1:667:A:LYS:HD2 | 6        | 7.57          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1 | 4        | 7.47          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2 | 4        | 7.47          |
| (1,7)    | 1:628:A:LEU:HD22 | 1:625:A:MET:HE3 | 5        | 7.47          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1 | 15       | 7.46          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2 | 15       | 7.46          |
| (1,482)  | 1:664:A:LEU:HD11 | 1:667:A:LYS:HD2 | 13       | 7.44          |
| (1,148)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE1 | 14       | 7.43          |
| (1,148)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE2 | 14       | 7.43          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,420)  | 1:635:A:VAL:HG13 | 1:634:A:LYS:HE2 | 8        | 7.41          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1 | 17       | 7.41          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2 | 17       | 7.41          |
| (1,482)  | 1:664:A:LEU:HD11 | 1:667:A:LYS:HD2 | 17       | 7.38          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1 | 16       | 7.34          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2 | 16       | 7.34          |
| (1,482)  | 1:664:A:LEU:HD11 | 1:667:A:LYS:HD2 | 8        | 7.33          |
| (1,148)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE1 | 2        | 7.32          |
| (1,148)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE2 | 2        | 7.32          |
| (1,148)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE1 | 20       | 7.32          |
| (1,148)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE2 | 20       | 7.32          |
| (1,7)    | 1:628:A:LEU:HD22 | 1:625:A:MET:HE2 | 1        | 7.31          |
| (1,1)    | 1:656:A:LYS:HE2  | 1:639:A:MET:HE3 | 3        | 7.26          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1 | 5        | 7.25          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2 | 5        | 7.25          |
| (1,482)  | 1:664:A:LEU:HD13 | 1:667:A:LYS:HD2 | 1        | 7.18          |
| (1,482)  | 1:664:A:LEU:HD11 | 1:667:A:LYS:HD2 | 4        | 7.17          |
| (1,1007) | 1:640:A:TYR:HA   | 1:591:A:TRP:HZ2 | 2        | 7.15          |
| (1,1)    | 1:656:A:LYS:HE2  | 1:639:A:MET:HE3 | 11       | 7.05          |
| (1,725)  | 1:591:A:TRP:HE1  | 1:589:A:LYS:HG3 | 15       | 7.02          |
| (1,482)  | 1:664:A:LEU:HD13 | 1:667:A:LYS:HD2 | 10       | 7.01          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1 | 8        | 6.98          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2 | 8        | 6.98          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1 | 13       | 6.94          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2 | 13       | 6.94          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1 | 6        | 6.87          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2 | 6        | 6.87          |
| (1,1)    | 1:656:A:LYS:HE2  | 1:639:A:MET:HE2 | 7        | 6.84          |
| (1,7)    | 1:628:A:LEU:HD23 | 1:625:A:MET:HE1 | 17       | 6.79          |
| (1,433)  | 1:656:A:LYS:HG2  | 1:639:A:MET:HE3 | 17       | 6.71          |
| (1,433)  | 1:656:A:LYS:HG2  | 1:639:A:MET:HE1 | 1        | 6.62          |
| (1,7)    | 1:628:A:LEU:HD21 | 1:625:A:MET:HE1 | 19       | 6.62          |
| (1,433)  | 1:656:A:LYS:HG2  | 1:639:A:MET:HE2 | 19       | 6.61          |
| (1,1014) | 1:591:A:TRP:HH2  | 1:640:A:TYR:HD1 | 2        | 6.59          |
| (1,1014) | 1:591:A:TRP:HH2  | 1:640:A:TYR:HD2 | 2        | 6.59          |
| (1,7)    | 1:628:A:LEU:HD22 | 1:625:A:MET:HE1 | 13       | 6.57          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1 | 10       | 6.56          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2 | 10       | 6.56          |
| (1,433)  | 1:656:A:LYS:HG2  | 1:639:A:MET:HE1 | 4        | 6.5           |
| (1,482)  | 1:664:A:LEU:HD13 | 1:667:A:LYS:HD2 | 14       | 6.49          |
| (1,7)    | 1:628:A:LEU:HD23 | 1:625:A:MET:HE1 | 10       | 6.39          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1 | 9        | 6.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2  | 9        | 6.38          |
| (1,7)    | 1:628:A:LEU:HD22 | 1:625:A:MET:HE2  | 12       | 6.36          |
| (1,1)    | 1:656:A:LYS:HE2  | 1:639:A:MET:HE1  | 20       | 6.34          |
| (1,420)  | 1:635:A:VAL:HG13 | 1:634:A:LYS:HE2  | 13       | 6.33          |
| (1,7)    | 1:628:A:LEU:HD21 | 1:625:A:MET:HE2  | 11       | 6.33          |
| (1,605)  | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD22 | 12       | 6.3           |
| (1,605)  | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD21 | 19       | 6.29          |
| (1,433)  | 1:656:A:LYS:HG2  | 1:639:A:MET:HE2  | 8        | 6.28          |
| (1,433)  | 1:656:A:LYS:HG2  | 1:639:A:MET:HE2  | 16       | 6.28          |
| (1,7)    | 1:628:A:LEU:HD21 | 1:625:A:MET:HE3  | 6        | 6.25          |
| (1,605)  | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD23 | 8        | 6.21          |
| (1,605)  | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD22 | 7        | 6.19          |
| (1,141)  | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE1  | 8        | 6.19          |
| (1,141)  | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE2  | 8        | 6.19          |
| (1,1)    | 1:656:A:LYS:HE2  | 1:639:A:MET:HE1  | 2        | 6.19          |
| (1,482)  | 1:664:A:LEU:HD11 | 1:667:A:LYS:HD2  | 9        | 6.18          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1  | 1        | 6.18          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2  | 1        | 6.18          |
| (1,1015) | 1:591:A:TRP:HH2  | 1:640:A:TYR:HE1  | 2        | 6.17          |
| (1,1015) | 1:591:A:TRP:HH2  | 1:640:A:TYR:HE2  | 2        | 6.17          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1  | 18       | 6.17          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2  | 18       | 6.17          |
| (1,605)  | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD22 | 11       | 6.16          |
| (1,7)    | 1:628:A:LEU:HD21 | 1:625:A:MET:HE2  | 15       | 6.16          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1  | 2        | 6.15          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2  | 2        | 6.15          |
| (1,7)    | 1:628:A:LEU:HD22 | 1:625:A:MET:HE2  | 8        | 6.15          |
| (1,605)  | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD22 | 6        | 6.13          |
| (1,1)    | 1:656:A:LYS:HE2  | 1:639:A:MET:HE3  | 17       | 6.13          |
| (1,141)  | 1:595:A:VAL:HG23 | 1:640:A:TYR:HE1  | 13       | 6.12          |
| (1,141)  | 1:595:A:VAL:HG23 | 1:640:A:TYR:HE2  | 13       | 6.12          |
| (1,605)  | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD22 | 4        | 6.1           |
| (1,141)  | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE1  | 10       | 6.1           |
| (1,141)  | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE2  | 10       | 6.1           |
| (1,420)  | 1:635:A:VAL:HG11 | 1:634:A:LYS:HE2  | 3        | 6.09          |
| (1,605)  | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD22 | 20       | 6.05          |
| (1,433)  | 1:656:A:LYS:HG2  | 1:639:A:MET:HE3  | 12       | 6.05          |
| (1,724)  | 1:591:A:TRP:HE1  | 1:589:A:LYS:HD2  | 15       | 6.01          |
| (1,433)  | 1:656:A:LYS:HG2  | 1:639:A:MET:HE2  | 20       | 6.01          |
| (1,1)    | 1:656:A:LYS:HE2  | 1:639:A:MET:HE3  | 1        | 5.96          |
| (1,420)  | 1:635:A:VAL:HG13 | 1:634:A:LYS:HE2  | 4        | 5.94          |
| (1,141)  | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE1  | 20       | 5.93          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,141) | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE2  | 20       | 5.93          |
| (1,420) | 1:635:A:VAL:HG11 | 1:634:A:LYS:HE2  | 7        | 5.91          |
| (1,109) | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1  | 7        | 5.89          |
| (1,109) | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2  | 7        | 5.89          |
| (1,605) | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD23 | 15       | 5.85          |
| (1,433) | 1:656:A:LYS:HG2  | 1:639:A:MET:HE2  | 18       | 5.85          |
| (1,605) | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD21 | 3        | 5.82          |
| (1,420) | 1:635:A:VAL:HG13 | 1:634:A:LYS:HE2  | 20       | 5.81          |
| (1,7)   | 1:628:A:LEU:HD23 | 1:625:A:MET:HE2  | 4        | 5.79          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 10       | 5.78          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 10       | 5.78          |
| (1,7)   | 1:628:A:LEU:HD21 | 1:625:A:MET:HE2  | 9        | 5.77          |
| (1,433) | 1:656:A:LYS:HG2  | 1:639:A:MET:HE1  | 3        | 5.75          |
| (1,434) | 1:635:A:VAL:HG23 | 1:639:A:MET:HE3  | 14       | 5.7           |
| (1,420) | 1:635:A:VAL:HG11 | 1:634:A:LYS:HE2  | 1        | 5.7           |
| (1,141) | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE1  | 6        | 5.69          |
| (1,141) | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE2  | 6        | 5.69          |
| (1,434) | 1:635:A:VAL:HG23 | 1:639:A:MET:HE3  | 4        | 5.64          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 20       | 5.63          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 20       | 5.63          |
| (1,434) | 1:635:A:VAL:HG21 | 1:639:A:MET:HE3  | 3        | 5.62          |
| (1,571) | 1:591:A:TRP:HD1  | 1:589:A:LYS:HA   | 15       | 5.61          |
| (1,141) | 1:595:A:VAL:HG23 | 1:640:A:TYR:HE1  | 17       | 5.61          |
| (1,141) | 1:595:A:VAL:HG23 | 1:640:A:TYR:HE2  | 17       | 5.61          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 17       | 5.61          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 8        | 5.6           |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 8        | 5.6           |
| (1,438) | 1:672:A:LEU:HD11 | 1:671:A:ARG:HG3  | 12       | 5.58          |
| (1,482) | 1:664:A:LEU:HD13 | 1:667:A:LYS:HD2  | 20       | 5.57          |
| (1,141) | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE1  | 11       | 5.56          |
| (1,141) | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE2  | 11       | 5.56          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 6        | 5.55          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 6        | 5.55          |
| (1,420) | 1:635:A:VAL:HG11 | 1:634:A:LYS:HE2  | 17       | 5.54          |
| (1,434) | 1:635:A:VAL:HG23 | 1:639:A:MET:HE1  | 20       | 5.53          |
| (1,433) | 1:656:A:LYS:HG2  | 1:639:A:MET:HE1  | 14       | 5.51          |
| (1,434) | 1:635:A:VAL:HG23 | 1:639:A:MET:HE1  | 16       | 5.48          |
| (1,724) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HD2  | 2        | 5.46          |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE1  | 8        | 5.42          |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE2  | 8        | 5.42          |
| (1,487) | 1:664:A:LEU:HD13 | 1:667:A:LYS:HG2  | 7        | 5.41          |
| (1,141) | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE1  | 15       | 5.41          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,141) | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE2  | 15       | 5.41          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 13       | 5.38          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 13       | 5.38          |
| (1,420) | 1:635:A:VAL:HG12 | 1:634:A:LYS:HE2  | 16       | 5.37          |
| (1,109) | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1  | 11       | 5.36          |
| (1,109) | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2  | 11       | 5.36          |
| (1,1)   | 1:656:A:LYS:HE2  | 1:639:A:MET:HE1  | 16       | 5.36          |
| (1,482) | 1:664:A:LEU:HD12 | 1:667:A:LYS:HD2  | 15       | 5.35          |
| (1,142) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE1  | 13       | 5.35          |
| (1,142) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE2  | 13       | 5.35          |
| (1,536) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD22 | 19       | 5.34          |
| (1,434) | 1:635:A:VAL:HG23 | 1:639:A:MET:HE2  | 7        | 5.34          |
| (1,420) | 1:635:A:VAL:HG13 | 1:634:A:LYS:HE2  | 2        | 5.33          |
| (1,1)   | 1:656:A:LYS:HE2  | 1:639:A:MET:HE3  | 4        | 5.33          |
| (1,725) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HG3  | 2        | 5.31          |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD22 | 6        | 5.31          |
| (1,434) | 1:635:A:VAL:HG23 | 1:639:A:MET:HE3  | 1        | 5.31          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 3        | 5.31          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 13       | 5.31          |
| (1,7)   | 1:628:A:LEU:HD22 | 1:625:A:MET:HE1  | 2        | 5.3           |
| (1,420) | 1:635:A:VAL:HG12 | 1:634:A:LYS:HE2  | 9        | 5.28          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 19       | 5.27          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 11       | 5.24          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 11       | 5.24          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 12       | 5.24          |
| (1,7)   | 1:628:A:LEU:HD23 | 1:625:A:MET:HE1  | 16       | 5.24          |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE1  | 10       | 5.23          |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE2  | 10       | 5.23          |
| (1,434) | 1:635:A:VAL:HG23 | 1:639:A:MET:HE1  | 2        | 5.22          |
| (1,433) | 1:656:A:LYS:HG2  | 1:639:A:MET:HE3  | 7        | 5.21          |
| (1,420) | 1:635:A:VAL:HG11 | 1:634:A:LYS:HE2  | 15       | 5.2           |
| (1,625) | 1:632:A:ALA:HB3  | 1:628:A:LEU:HD11 | 14       | 5.17          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD11 | 16       | 5.17          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD11 | 16       | 5.17          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 17       | 5.15          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 17       | 5.15          |
| (1,487) | 1:664:A:LEU:HD13 | 1:667:A:LYS:HG2  | 1        | 5.13          |
| (1,487) | 1:664:A:LEU:HD13 | 1:667:A:LYS:HG2  | 20       | 5.12          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 15       | 5.11          |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE1  | 19       | 5.08          |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE2  | 19       | 5.08          |
| (1,142) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE1  | 17       | 5.08          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,142) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE2  | 17       | 5.08          |
| (1,433) | 1:656:A:LYS:HG2  | 1:639:A:MET:HE1  | 2        | 5.07          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD21 | 19       | 5.07          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 15       | 5.07          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 15       | 5.07          |
| (1,142) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HE1  | 20       | 5.05          |
| (1,142) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HE2  | 20       | 5.05          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 5        | 5.05          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD1  | 14       | 5.04          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD2  | 14       | 5.04          |
| (1,482) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HD2  | 2        | 5.04          |
| (1,109) | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1  | 20       | 5.04          |
| (1,109) | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2  | 20       | 5.04          |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE1  | 6        | 5.02          |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE2  | 6        | 5.02          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD1  | 20       | 4.99          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD2  | 20       | 4.99          |
| (1,487) | 1:664:A:LEU:HD12 | 1:667:A:LYS:HG2  | 15       | 4.98          |
| (1,482) | 1:664:A:LEU:HD12 | 1:667:A:LYS:HD2  | 11       | 4.97          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD1  | 2        | 4.96          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD2  | 2        | 4.96          |
| (1,7)   | 1:628:A:LEU:HD23 | 1:625:A:MET:HE3  | 20       | 4.95          |
| (1,487) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HG2  | 13       | 4.89          |
| (1,142) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE1  | 11       | 4.89          |
| (1,142) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE2  | 11       | 4.89          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 16       | 4.88          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD13 | 15       | 4.86          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD13 | 15       | 4.86          |
| (1,482) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HD2  | 19       | 4.85          |
| (1,487) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HG2  | 12       | 4.84          |
| (1,434) | 1:635:A:VAL:HG23 | 1:639:A:MET:HE3  | 17       | 4.84          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 8        | 4.84          |
| (1,625) | 1:632:A:ALA:HB3  | 1:628:A:LEU:HD13 | 19       | 4.83          |
| (1,487) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HG2  | 17       | 4.82          |
| (1,7)   | 1:628:A:LEU:HD23 | 1:625:A:MET:HE2  | 14       | 4.82          |
| (1,1)   | 1:656:A:LYS:HE2  | 1:639:A:MET:HE1  | 19       | 4.82          |
| (1,487) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HG2  | 6        | 4.81          |
| (1,142) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HE1  | 15       | 4.81          |
| (1,142) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HE2  | 15       | 4.81          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 10       | 4.81          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD22 | 13       | 4.79          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD21 | 19       | 4.79          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,434)  | 1:635:A:VAL:HG23 | 1:639:A:MET:HE2  | 8        | 4.79          |
| (1,500)  | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD22 | 5        | 4.77          |
| (1,627)  | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD21 | 15       | 4.74          |
| (1,39)   | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 9        | 4.72          |
| (1,1)    | 1:656:A:LYS:HE2  | 1:639:A:MET:HE2  | 8        | 4.72          |
| (1,594)  | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG13 | 8        | 4.71          |
| (1,487)  | 1:664:A:LEU:HD11 | 1:667:A:LYS:HG2  | 8        | 4.71          |
| (1,929)  | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 11       | 4.7           |
| (1,482)  | 1:664:A:LEU:HD11 | 1:667:A:LYS:HD2  | 3        | 4.69          |
| (1,627)  | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD23 | 10       | 4.67          |
| (1,39)   | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 6        | 4.67          |
| (1,39)   | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 1        | 4.64          |
| (1,625)  | 1:632:A:ALA:HB3  | 1:628:A:LEU:HD11 | 10       | 4.63          |
| (1,470)  | 1:635:A:VAL:HG11 | 1:639:A:MET:HE1  | 19       | 4.63          |
| (1,626)  | 1:625:A:MET:HE1  | 1:628:A:LEU:HD12 | 17       | 4.59          |
| (1,369)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD23 | 1        | 4.58          |
| (1,144)  | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 20       | 4.56          |
| (1,144)  | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 20       | 4.56          |
| (1,5)    | 1:608:A:VAL:HG23 | 1:625:A:MET:HE2  | 7        | 4.55          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 2        | 4.54          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 2        | 4.54          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 2        | 4.54          |
| (1,434)  | 1:635:A:VAL:HG21 | 1:639:A:MET:HE3  | 11       | 4.54          |
| (1,1)    | 1:656:A:LYS:HE2  | 1:639:A:MET:HE1  | 6        | 4.52          |
| (1,144)  | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 10       | 4.51          |
| (1,144)  | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 10       | 4.51          |
| (1,487)  | 1:664:A:LEU:HD11 | 1:667:A:LYS:HG2  | 4        | 4.5           |
| (1,482)  | 1:664:A:LEU:HD12 | 1:667:A:LYS:HD2  | 16       | 4.5           |
| (1,148)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE1  | 10       | 4.49          |
| (1,148)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE2  | 10       | 4.49          |
| (1,627)  | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD21 | 11       | 4.48          |
| (1,898)  | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 18       | 4.47          |
| (1,628)  | 1:608:A:VAL:HA   | 1:628:A:LEU:HD23 | 15       | 4.46          |
| (1,625)  | 1:632:A:ALA:HB2  | 1:628:A:LEU:HD11 | 13       | 4.46          |
| (1,625)  | 1:632:A:ALA:HB1  | 1:628:A:LEU:HD13 | 4        | 4.44          |
| (1,625)  | 1:632:A:ALA:HB2  | 1:628:A:LEU:HD12 | 18       | 4.44          |
| (1,929)  | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 10       | 4.43          |
| (1,625)  | 1:632:A:ALA:HB2  | 1:628:A:LEU:HD13 | 16       | 4.42          |
| (1,535)  | 1:639:A:MET:HG3  | 1:653:A:LEU:HD22 | 1        | 4.41          |
| (1,171)  | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 7        | 4.41          |
| (1,627)  | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD22 | 5        | 4.38          |
| (1,625)  | 1:632:A:ALA:HB2  | 1:628:A:LEU:HD12 | 15       | 4.38          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,482) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HD2  | 18       | 4.38          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD12 | 18       | 4.38          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD12 | 18       | 4.38          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD21 | 11       | 4.37          |
| (3,8)   | 1:612:A:PHE:HE1  | 2:546:B:LEU:HA   | 7        | 4.35          |
| (3,8)   | 1:612:A:PHE:HE2  | 2:546:B:LEU:HA   | 7        | 4.35          |
| (1,536) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD23 | 8        | 4.35          |
| (1,536) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD21 | 11       | 4.34          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 19       | 4.33          |
| (1,625) | 1:632:A:ALA:HB3  | 1:628:A:LEU:HD11 | 17       | 4.32          |
| (1,482) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HD2  | 5        | 4.32          |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD23 | 10       | 4.31          |
| (1,594) | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG11 | 15       | 4.31          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 18       | 4.31          |
| (1,625) | 1:632:A:ALA:HB1  | 1:628:A:LEU:HD12 | 1        | 4.3           |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD21 | 19       | 4.3           |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 3        | 4.29          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 1        | 4.27          |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 19       | 4.26          |
| (1,640) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD11 | 5        | 4.26          |
| (1,470) | 1:635:A:VAL:HG13 | 1:639:A:MET:HE3  | 12       | 4.26          |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD22 | 1        | 4.25          |
| (1,625) | 1:632:A:ALA:HB3  | 1:628:A:LEU:HD11 | 20       | 4.25          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD23 | 1        | 4.25          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 6        | 4.25          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 6        | 4.25          |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD22 | 13       | 4.24          |
| (1,625) | 1:632:A:ALA:HB2  | 1:628:A:LEU:HD12 | 5        | 4.23          |
| (1,625) | 1:632:A:ALA:HB3  | 1:628:A:LEU:HD12 | 8        | 4.23          |
| (1,594) | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG11 | 13       | 4.23          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD13 | 12       | 4.22          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD13 | 12       | 4.22          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 10       | 4.21          |
| (1,640) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD13 | 14       | 4.21          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 19       | 4.21          |
| (1,433) | 1:656:A:LYS:HG2  | 1:639:A:MET:HE3  | 11       | 4.21          |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD1  | 16       | 4.21          |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD2  | 16       | 4.21          |
| (1,626) | 1:625:A:MET:HE2  | 1:628:A:LEU:HD11 | 7        | 4.2           |
| (1,625) | 1:632:A:ALA:HB1  | 1:628:A:LEU:HD11 | 2        | 4.19          |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD21 | 9        | 4.18          |
| (1,536) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD22 | 7        | 4.18          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,438) | 1:672:A:LEU:HD13 | 1:671:A:ARG:HG3  | 14       | 4.17          |
| (1,626) | 1:625:A:MET:HE3  | 1:628:A:LEU:HD13 | 18       | 4.15          |
| (1,625) | 1:632:A:ALA:HB1  | 1:628:A:LEU:HD11 | 9        | 4.15          |
| (1,536) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD23 | 2        | 4.15          |
| (1,487) | 1:664:A:LEU:HD13 | 1:667:A:LYS:HG2  | 14       | 4.15          |
| (1,438) | 1:672:A:LEU:HD12 | 1:671:A:ARG:HG3  | 15       | 4.15          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD23 | 11       | 4.13          |
| (1,1)   | 1:656:A:LYS:HE2  | 1:639:A:MET:HE3  | 13       | 4.13          |
| (3,7)   | 1:612:A:PHE:HE1  | 2:546:B:LEU:HD21 | 7        | 4.12          |
| (3,7)   | 1:612:A:PHE:HE1  | 2:546:B:LEU:HD22 | 7        | 4.12          |
| (3,7)   | 1:612:A:PHE:HE1  | 2:546:B:LEU:HD23 | 7        | 4.12          |
| (3,7)   | 1:612:A:PHE:HE2  | 2:546:B:LEU:HD21 | 7        | 4.12          |
| (3,7)   | 1:612:A:PHE:HE2  | 2:546:B:LEU:HD22 | 7        | 4.12          |
| (3,7)   | 1:612:A:PHE:HE2  | 2:546:B:LEU:HD23 | 7        | 4.12          |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD21 | 6        | 4.12          |
| (1,626) | 1:625:A:MET:HE2  | 1:628:A:LEU:HD13 | 3        | 4.11          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD23 | 8        | 4.11          |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD23 | 18       | 4.1           |
| (1,438) | 1:672:A:LEU:HD11 | 1:671:A:ARG:HG3  | 10       | 4.1           |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD23 | 4        | 4.08          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 1        | 4.08          |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG22 | 8        | 4.08          |
| (1,535) | 1:639:A:MET:HG3  | 1:653:A:LEU:HD21 | 19       | 4.07          |
| (1,487) | 1:664:A:LEU:HD13 | 1:667:A:LYS:HG2  | 10       | 4.07          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD23 | 3        | 4.06          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 5        | 4.04          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 11       | 4.01          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 11       | 4.01          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 20       | 4.01          |
| (1,594) | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG12 | 9        | 4.0           |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 6        | 3.99          |
| (1,438) | 1:672:A:LEU:HD11 | 1:671:A:ARG:HG3  | 1        | 3.99          |
| (1,438) | 1:672:A:LEU:HD13 | 1:671:A:ARG:HG3  | 2        | 3.99          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD23 | 3        | 3.99          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 4        | 3.98          |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD23 | 17       | 3.98          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 14       | 3.98          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 5        | 3.97          |
| (1,438) | 1:672:A:LEU:HD11 | 1:671:A:ARG:HG3  | 17       | 3.97          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD23 | 2        | 3.97          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD22 | 20       | 3.96          |
| (1,626) | 1:625:A:MET:HE3  | 1:628:A:LEU:HD13 | 5        | 3.95          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,547) | 1:603:A:LEU:HD12 | 1:606:A:LYS:HD2  | 9        | 3.94          |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD21 | 11       | 3.94          |
| (1,438) | 1:672:A:LEU:HD12 | 1:671:A:ARG:HG3  | 4        | 3.94          |
| (1,438) | 1:672:A:LEU:HD11 | 1:671:A:ARG:HG3  | 19       | 3.94          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 11       | 3.93          |
| (1,625) | 1:632:A:ALA:HB1  | 1:628:A:LEU:HD11 | 12       | 3.93          |
| (1,594) | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG13 | 4        | 3.93          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 13       | 3.93          |
| (1,438) | 1:672:A:LEU:HD12 | 1:671:A:ARG:HG3  | 11       | 3.93          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 9        | 3.92          |
| (1,524) | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD3  | 1        | 3.92          |
| (1,5)   | 1:608:A:VAL:HG22 | 1:625:A:MET:HE1  | 13       | 3.92          |
| (1,640) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD11 | 4        | 3.9           |
| (1,594) | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG13 | 2        | 3.9           |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 9        | 3.9           |
| (1,438) | 1:672:A:LEU:HD13 | 1:671:A:ARG:HG3  | 18       | 3.9           |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD23 | 11       | 3.89          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 15       | 3.89          |
| (1,524) | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD3  | 3        | 3.89          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD22 | 15       | 3.89          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 6        | 3.88          |
| (1,524) | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD3  | 2        | 3.88          |
| (1,438) | 1:672:A:LEU:HD13 | 1:671:A:ARG:HG3  | 6        | 3.88          |
| (1,438) | 1:672:A:LEU:HD13 | 1:671:A:ARG:HG3  | 13       | 3.88          |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD22 | 8        | 3.87          |
| (1,524) | 1:595:A:VAL:HG23 | 1:646:A:ARG:HD3  | 11       | 3.87          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD21 | 12       | 3.87          |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD22 | 2        | 3.86          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 2        | 3.86          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 17       | 3.86          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 20       | 3.85          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 8        | 3.85          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 8        | 3.85          |
| (1,1)   | 1:656:A:LYS:HE2  | 1:639:A:MET:HE3  | 12       | 3.85          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 10       | 3.84          |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 14       | 3.83          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 8        | 3.83          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 16       | 3.83          |
| (1,626) | 1:625:A:MET:HE2  | 1:628:A:LEU:HD13 | 1        | 3.82          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 3        | 3.82          |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD22 | 12       | 3.81          |
| (1,438) | 1:672:A:LEU:HD11 | 1:671:A:ARG:HG3  | 20       | 3.81          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,961) | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 1        | 3.8           |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 13       | 3.8           |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 11       | 3.8           |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD23 | 8        | 3.8           |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD21 | 6        | 3.79          |
| (1,547) | 1:603:A:LEU:HD12 | 1:606:A:LYS:HD2  | 20       | 3.79          |
| (1,487) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HG2  | 5        | 3.79          |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD22 | 19       | 3.77          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD21 | 8        | 3.77          |
| (1,487) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HG2  | 19       | 3.76          |
| (1,420) | 1:635:A:VAL:HG12 | 1:634:A:LYS:HE2  | 10       | 3.76          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 13       | 3.75          |
| (1,535) | 1:639:A:MET:HG3  | 1:653:A:LEU:HD21 | 11       | 3.75          |
| (1,524) | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD3  | 17       | 3.75          |
| (1,480) | 1:653:A:LEU:HD23 | 1:636:A:GLU:HA   | 1        | 3.75          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 16       | 3.74          |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD22 | 20       | 3.74          |
| (1,420) | 1:635:A:VAL:HG12 | 1:634:A:LYS:HE2  | 6        | 3.74          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD22 | 7        | 3.74          |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD21 | 4        | 3.73          |
| (1,535) | 1:639:A:MET:HG3  | 1:653:A:LEU:HD22 | 20       | 3.73          |
| (1,524) | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD3  | 9        | 3.73          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 17       | 3.72          |
| (1,492) | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 5        | 3.72          |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 7        | 3.71          |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD22 | 5        | 3.71          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 7        | 3.7           |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 20       | 3.7           |
| (1,640) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD12 | 13       | 3.7           |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 6        | 3.69          |
| (1,547) | 1:603:A:LEU:HD13 | 1:606:A:LYS:HD2  | 8        | 3.69          |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD21 | 20       | 3.68          |
| (1,492) | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 4        | 3.68          |
| (1,487) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HG2  | 9        | 3.68          |
| (1,470) | 1:635:A:VAL:HG13 | 1:639:A:MET:HE2  | 18       | 3.68          |
| (1,6)   | 1:608:A:VAL:HG13 | 1:625:A:MET:HE2  | 7        | 3.68          |
| (1,438) | 1:672:A:LEU:HD13 | 1:671:A:ARG:HG3  | 16       | 3.67          |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG23 | 10       | 3.66          |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD22 | 18       | 3.65          |
| (1,626) | 1:625:A:MET:HE1  | 1:628:A:LEU:HD11 | 19       | 3.65          |
| (1,594) | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG12 | 16       | 3.65          |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD21 | 1        | 3.64          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,524) | 1:595:A:VAL:HG23 | 1:646:A:ARG:HD3  | 15       | 3.64          |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG23 | 17       | 3.64          |
| (1,536) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD23 | 1        | 3.63          |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD22 | 1        | 3.62          |
| (1,605) | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD23 | 2        | 3.62          |
| (1,4)   | 1:629:A:VAL:HG23 | 1:625:A:MET:HE2  | 19       | 3.62          |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD23 | 2        | 3.61          |
| (1,487) | 1:664:A:LEU:HD12 | 1:667:A:LYS:HG2  | 16       | 3.61          |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD23 | 7        | 3.6           |
| (1,594) | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG11 | 3        | 3.6           |
| (1,487) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HG2  | 18       | 3.6           |
| (1,420) | 1:635:A:VAL:HG13 | 1:634:A:LYS:HE2  | 18       | 3.6           |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 17       | 3.6           |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 17       | 3.6           |
| (1,4)   | 1:629:A:VAL:HG22 | 1:625:A:MET:HE3  | 1        | 3.6           |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 17       | 3.59          |
| (1,487) | 1:664:A:LEU:HD12 | 1:667:A:LYS:HG2  | 11       | 3.59          |
| (1,477) | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG21 | 1        | 3.59          |
| (1,420) | 1:635:A:VAL:HG13 | 1:634:A:LYS:HE2  | 14       | 3.59          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD22 | 17       | 3.59          |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD23 | 12       | 3.58          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE1  | 5        | 3.58          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE2  | 5        | 3.58          |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 2        | 3.57          |
| (1,625) | 1:632:A:ALA:HB1  | 1:628:A:LEU:HD11 | 11       | 3.57          |
| (1,438) | 1:672:A:LEU:HD12 | 1:671:A:ARG:HG3  | 7        | 3.57          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 13       | 3.57          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 13       | 3.57          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 15       | 3.57          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 15       | 3.57          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 2        | 3.56          |
| (1,5)   | 1:608:A:VAL:HG22 | 1:625:A:MET:HE3  | 20       | 3.56          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 7        | 3.55          |
| (1,438) | 1:672:A:LEU:HD11 | 1:671:A:ARG:HG3  | 5        | 3.55          |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE1  | 11       | 3.55          |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE2  | 11       | 3.55          |
| (1,1)   | 1:656:A:LYS:HE2  | 1:639:A:MET:HE3  | 10       | 3.55          |
| (1,594) | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG11 | 17       | 3.54          |
| (1,438) | 1:672:A:LEU:HD11 | 1:671:A:ARG:HG3  | 3        | 3.54          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 12       | 3.53          |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD23 | 18       | 3.53          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD21 | 15       | 3.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,226)  | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG21 | 18       | 3.53          |
| (1,1)    | 1:656:A:LYS:HE2  | 1:639:A:MET:HE2  | 18       | 3.53          |
| (2,104)  | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 12       | 3.52          |
| (1,627)  | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD23 | 17       | 3.52          |
| (1,608)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD22 | 2        | 3.52          |
| (1,898)  | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 15       | 3.51          |
| (1,608)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD21 | 8        | 3.5           |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD1  | 11       | 3.5           |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD2  | 11       | 3.5           |
| (1,433)  | 1:656:A:LYS:HG2  | 1:639:A:MET:HE2  | 9        | 3.5           |
| (1,4)    | 1:629:A:VAL:HG21 | 1:625:A:MET:HE1  | 5        | 3.5           |
| (1,628)  | 1:608:A:VAL:HA   | 1:628:A:LEU:HD22 | 13       | 3.49          |
| (1,226)  | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG21 | 3        | 3.49          |
| (1,547)  | 1:603:A:LEU:HD11 | 1:606:A:LYS:HD2  | 2        | 3.48          |
| (1,226)  | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG22 | 6        | 3.48          |
| (1,148)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE1  | 7        | 3.48          |
| (1,148)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE2  | 7        | 3.48          |
| (1,547)  | 1:603:A:LEU:HD12 | 1:606:A:LYS:HD2  | 13       | 3.47          |
| (1,534)  | 1:639:A:MET:HG2  | 1:653:A:LEU:HD22 | 7        | 3.47          |
| (1,420)  | 1:635:A:VAL:HG11 | 1:634:A:LYS:HE2  | 19       | 3.47          |
| (2,105)  | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 5        | 3.46          |
| (1,929)  | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 8        | 3.46          |
| (1,535)  | 1:639:A:MET:HG3  | 1:653:A:LEU:HD23 | 3        | 3.46          |
| (1,5)    | 1:608:A:VAL:HG23 | 1:625:A:MET:HE1  | 5        | 3.46          |
| (1,961)  | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 11       | 3.45          |
| (1,929)  | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 16       | 3.45          |
| (1,629)  | 1:625:A:MET:HA   | 1:628:A:LEU:HD21 | 5        | 3.45          |
| (1,628)  | 1:608:A:VAL:HA   | 1:628:A:LEU:HD23 | 4        | 3.45          |
| (1,535)  | 1:639:A:MET:HG3  | 1:653:A:LEU:HD23 | 8        | 3.45          |
| (1,628)  | 1:608:A:VAL:HA   | 1:628:A:LEU:HD21 | 9        | 3.44          |
| (1,357)  | 1:608:A:VAL:HG23 | 1:629:A:VAL:HA   | 17       | 3.43          |
| (1,5)    | 1:608:A:VAL:HG22 | 1:625:A:MET:HE2  | 19       | 3.43          |
| (1,535)  | 1:639:A:MET:HG3  | 1:653:A:LEU:HD23 | 2        | 3.42          |
| (1,438)  | 1:672:A:LEU:HD11 | 1:671:A:ARG:HG3  | 9        | 3.42          |
| (2,105)  | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 1        | 3.41          |
| (1,534)  | 1:639:A:MET:HG2  | 1:653:A:LEU:HD23 | 3        | 3.41          |
| (2,105)  | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 11       | 3.4           |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 15       | 3.4           |
| (1,628)  | 1:608:A:VAL:HA   | 1:628:A:LEU:HD21 | 11       | 3.4           |
| (1,567)  | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 7        | 3.4           |
| (1,632)  | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 11       | 3.39          |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG21 | 19       | 3.39          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD1  | 12       | 3.39          |
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD2  | 12       | 3.39          |
| (1,4)   | 1:629:A:VAL:HG21 | 1:625:A:MET:HE1  | 18       | 3.39          |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 18       | 3.38          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 4        | 3.38          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE1  | 16       | 3.38          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE2  | 16       | 3.38          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 4        | 3.37          |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD23 | 16       | 3.37          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD21 | 6        | 3.37          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD23 | 9        | 3.36          |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 10       | 3.35          |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD22 | 4        | 3.35          |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD23 | 20       | 3.35          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE1  | 15       | 3.35          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE2  | 15       | 3.35          |
| (1,961) | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 18       | 3.34          |
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD1  | 15       | 3.34          |
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD2  | 15       | 3.34          |
| (1,547) | 1:603:A:LEU:HD12 | 1:606:A:LYS:HD2  | 16       | 3.33          |
| (1,477) | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG23 | 14       | 3.33          |
| (1,4)   | 1:629:A:VAL:HG23 | 1:625:A:MET:HE2  | 17       | 3.33          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD21 | 16       | 3.32          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 11       | 3.3           |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD23 | 20       | 3.3           |
| (1,492) | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 16       | 3.3           |
| (1,430) | 1:664:A:LEU:HD21 | 1:661:A:GLN:HA   | 18       | 3.3           |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG23 | 15       | 3.3           |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD22 | 2        | 3.29          |
| (1,626) | 1:625:A:MET:HE3  | 1:628:A:LEU:HD13 | 6        | 3.29          |
| (1,961) | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 19       | 3.28          |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 14       | 3.28          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD11 | 13       | 3.28          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD11 | 13       | 3.28          |
| (1,547) | 1:603:A:LEU:HD13 | 1:606:A:LYS:HD2  | 7        | 3.28          |
| (1,492) | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 13       | 3.28          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD13 | 8        | 3.28          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD13 | 8        | 3.28          |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 3        | 3.27          |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD23 | 14       | 3.27          |
| (1,626) | 1:625:A:MET:HE1  | 1:628:A:LEU:HD12 | 13       | 3.27          |
| (1,547) | 1:603:A:LEU:HD13 | 1:606:A:LYS:HD2  | 1        | 3.27          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD21 | 2        | 3.26          |
| (1,620) | 1:625:A:MET:HG2  | 1:620:A:LEU:HD12 | 13       | 3.26          |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD21 | 3        | 3.26          |
| (1,482) | 1:664:A:LEU:HD13 | 1:667:A:LYS:HD2  | 7        | 3.26          |
| (1,477) | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG21 | 18       | 3.26          |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD13 | 15       | 3.26          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE1  | 8        | 3.25          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE2  | 8        | 3.25          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE1  | 8        | 3.25          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE2  | 8        | 3.25          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE1  | 8        | 3.25          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE2  | 8        | 3.25          |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 16       | 3.25          |
| (1,620) | 1:625:A:MET:HG2  | 1:620:A:LEU:HD13 | 10       | 3.25          |
| (1,961) | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 6        | 3.23          |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD21 | 15       | 3.23          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD23 | 14       | 3.23          |
| (1,484) | 1:607:A:LEU:HD22 | 1:653:A:LEU:HB2  | 10       | 3.23          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB1  | 15       | 3.23          |
| (1,39)  | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 4        | 3.23          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE1  | 9        | 3.22          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE2  | 9        | 3.22          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE1  | 9        | 3.22          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE2  | 9        | 3.22          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE1  | 9        | 3.22          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE2  | 9        | 3.22          |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD21 | 8        | 3.22          |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD22 | 1        | 3.22          |
| (1,6)   | 1:608:A:VAL:HG13 | 1:625:A:MET:HE2  | 17       | 3.22          |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD22 | 8        | 3.21          |
| (1,625) | 1:632:A:ALA:HB1  | 1:628:A:LEU:HD12 | 6        | 3.21          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD11 | 13       | 3.21          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD11 | 14       | 3.21          |
| (1,524) | 1:595:A:VAL:HG23 | 1:646:A:ARG:HD3  | 8        | 3.21          |
| (1,430) | 1:664:A:LEU:HD23 | 1:661:A:GLN:HA   | 12       | 3.21          |
| (1,495) | 1:653:A:LEU:HD12 | 1:603:A:LEU:HD11 | 18       | 3.2           |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD21 | 10       | 3.2           |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE1  | 5        | 3.19          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE2  | 5        | 3.19          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE1  | 5        | 3.19          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE2  | 5        | 3.19          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE1  | 5        | 3.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,28)   | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE2  | 5        | 3.19          |
| (3,28)   | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE1  | 18       | 3.19          |
| (3,28)   | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE2  | 18       | 3.19          |
| (3,28)   | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE1  | 18       | 3.19          |
| (3,28)   | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE2  | 18       | 3.19          |
| (3,28)   | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE1  | 18       | 3.19          |
| (3,28)   | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE2  | 18       | 3.19          |
| (1,961)  | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 10       | 3.19          |
| (1,628)  | 1:608:A:VAL:HA   | 1:628:A:LEU:HD22 | 12       | 3.19          |
| (2,105)  | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 19       | 3.18          |
| (1,961)  | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 8        | 3.18          |
| (1,605)  | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD23 | 13       | 3.18          |
| (1,500)  | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD23 | 18       | 3.18          |
| (1,500)  | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD21 | 20       | 3.18          |
| (1,119)  | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD11 | 7        | 3.18          |
| (1,119)  | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD11 | 7        | 3.18          |
| (1,24)   | 1:650:A:TYR:HA   | 1:653:A:LEU:HD11 | 16       | 3.18          |
| (1,929)  | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 7        | 3.17          |
| (1,898)  | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 8        | 3.17          |
| (1,622)  | 1:608:A:VAL:HA   | 1:628:A:LEU:HD12 | 10       | 3.17          |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD13 | 16       | 3.17          |
| (1,535)  | 1:639:A:MET:HG3  | 1:653:A:LEU:HD22 | 7        | 3.17          |
| (1,357)  | 1:608:A:VAL:HG22 | 1:629:A:VAL:HA   | 7        | 3.17          |
| (1,226)  | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG22 | 1        | 3.17          |
| (1,226)  | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG23 | 13       | 3.17          |
| (2,105)  | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 20       | 3.16          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 6        | 3.16          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 6        | 3.16          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 6        | 3.16          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 6        | 3.16          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 6        | 3.16          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 6        | 3.16          |
| (1,632)  | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 16       | 3.16          |
| (1,629)  | 1:625:A:MET:HA   | 1:628:A:LEU:HD21 | 12       | 3.16          |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG21 | 4        | 3.16          |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG22 | 12       | 3.16          |
| (1,961)  | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 20       | 3.15          |
| (1,927)  | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 6        | 3.15          |
| (1,601)  | 1:595:A:VAL:HG11 | 1:640:A:TYR:HD1  | 8        | 3.15          |
| (1,601)  | 1:595:A:VAL:HG11 | 1:640:A:TYR:HD2  | 8        | 3.15          |
| (1,626)  | 1:625:A:MET:HE2  | 1:628:A:LEU:HD12 | 11       | 3.14          |
| (3,28)   | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE1  | 1        | 3.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE2  | 1        | 3.13          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE1  | 1        | 3.13          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE2  | 1        | 3.13          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE1  | 1        | 3.13          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE2  | 1        | 3.13          |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD23 | 9        | 3.13          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD12 | 6        | 3.13          |
| (1,430) | 1:664:A:LEU:HD23 | 1:661:A:GLN:HA   | 11       | 3.13          |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 4        | 3.12          |
| (1,477) | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG22 | 7        | 3.12          |
| (1,927) | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 8        | 3.11          |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD22 | 19       | 3.11          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD12 | 17       | 3.11          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD12 | 17       | 3.11          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD13 | 4        | 3.09          |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG22 | 2        | 3.09          |
| (1,20)  | 1:660:A:ILE:HG22 | 1:664:A:LEU:HD22 | 19       | 3.09          |
| (1,679) | 1:643:A:ALA:H    | 1:652:A:LEU:HD22 | 10       | 3.08          |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD22 | 17       | 3.08          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 18       | 3.07          |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 2        | 3.07          |
| (1,601) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HD1  | 10       | 3.07          |
| (1,601) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HD2  | 10       | 3.07          |
| (1,927) | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 2        | 3.06          |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD23 | 11       | 3.06          |
| (1,626) | 1:625:A:MET:HE2  | 1:628:A:LEU:HD12 | 12       | 3.06          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD13 | 15       | 3.06          |
| (1,605) | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD22 | 17       | 3.06          |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 8        | 3.05          |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 1        | 3.05          |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 15       | 3.05          |
| (1,605) | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD23 | 18       | 3.05          |
| (1,435) | 1:653:A:LEU:HD13 | 1:639:A:MET:HE1  | 6        | 3.05          |
| (1,116) | 1:653:A:LEU:HD12 | 1:650:A:TYR:HD1  | 18       | 3.05          |
| (1,116) | 1:653:A:LEU:HD12 | 1:650:A:TYR:HD2  | 18       | 3.05          |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD12 | 18       | 3.05          |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 3        | 3.04          |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 14       | 3.04          |
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD12 | 18       | 3.04          |
| (1,480) | 1:653:A:LEU:HD22 | 1:636:A:GLU:HA   | 20       | 3.04          |
| (1,430) | 1:664:A:LEU:HD22 | 1:661:A:GLN:HA   | 14       | 3.04          |
| (1,679) | 1:643:A:ALA:H    | 1:652:A:LEU:HD23 | 14       | 3.03          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 7        | 3.03          |
| (1,487) | 1:664:A:LEU:HD11 | 1:667:A:LYS:HG2  | 2        | 3.03          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE1  | 17       | 3.02          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE2  | 17       | 3.02          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE1  | 17       | 3.02          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE2  | 17       | 3.02          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE1  | 17       | 3.02          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE2  | 17       | 3.02          |
| (1,961) | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 14       | 3.02          |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 5        | 3.02          |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 13       | 3.02          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 14       | 3.02          |
| (1,523) | 1:595:A:VAL:HG23 | 1:646:A:ARG:HD2  | 11       | 3.02          |
| (1,171) | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 19       | 3.02          |
| (1,927) | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 20       | 3.01          |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD23 | 14       | 3.01          |
| (1,547) | 1:603:A:LEU:HD13 | 1:606:A:LYS:HD2  | 14       | 3.01          |
| (1,496) | 1:599:A:LEU:HD12 | 1:603:A:LEU:HD23 | 17       | 3.01          |
| (1,430) | 1:664:A:LEU:HD23 | 1:661:A:GLN:HA   | 8        | 3.01          |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG22 | 7        | 3.01          |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG22 | 20       | 3.01          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 20       | 3.0           |
| (1,961) | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 5        | 3.0           |
| (1,927) | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 13       | 3.0           |
| (1,679) | 1:643:A:ALA:H    | 1:652:A:LEU:HD21 | 2        | 3.0           |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 4        | 3.0           |
| (1,617) | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 4        | 3.0           |
| (1,547) | 1:603:A:LEU:HD11 | 1:606:A:LYS:HD2  | 3        | 3.0           |
| (1,547) | 1:603:A:LEU:HD11 | 1:606:A:LYS:HD2  | 6        | 3.0           |
| (1,524) | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD3  | 19       | 3.0           |
| (1,430) | 1:664:A:LEU:HD21 | 1:661:A:GLN:HA   | 6        | 3.0           |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 17       | 2.99          |
| (1,601) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD1  | 13       | 2.99          |
| (1,601) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD2  | 13       | 2.99          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD23 | 17       | 2.99          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD11 | 13       | 2.99          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD11 | 13       | 2.99          |
| (1,20)  | 1:660:A:ILE:HG23 | 1:664:A:LEU:HD22 | 18       | 2.99          |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 9        | 2.98          |
| (1,679) | 1:643:A:ALA:H    | 1:652:A:LEU:HD21 | 6        | 2.98          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD13 | 16       | 2.98          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 12       | 2.98          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,480) | 1:653:A:LEU:HD21 | 1:636:A:GLU:HA   | 19       | 2.98          |
| (1,430) | 1:664:A:LEU:HD22 | 1:661:A:GLN:HA   | 4        | 2.98          |
| (1,420) | 1:635:A:VAL:HG11 | 1:634:A:LYS:HE2  | 11       | 2.98          |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 18       | 2.97          |
| (1,738) | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 4        | 2.97          |
| (1,679) | 1:643:A:ALA:H    | 1:652:A:LEU:HD23 | 11       | 2.97          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD11 | 9        | 2.97          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB3  | 16       | 2.97          |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 19       | 2.96          |
| (1,610) | 1:599:A:LEU:HD23 | 1:603:A:LEU:HD23 | 16       | 2.96          |
| (1,492) | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 15       | 2.96          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD13 | 5        | 2.96          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD13 | 5        | 2.96          |
| (1,117) | 1:653:A:LEU:HD21 | 1:650:A:TYR:HD1  | 14       | 2.96          |
| (1,117) | 1:653:A:LEU:HD21 | 1:650:A:TYR:HD2  | 14       | 2.96          |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 9        | 2.95          |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 9        | 2.95          |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 12       | 2.95          |
| (1,547) | 1:603:A:LEU:HD12 | 1:606:A:LYS:HD2  | 10       | 2.95          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB2  | 7        | 2.95          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 5        | 2.94          |
| (1,659) | 1:652:A:LEU:HB3  | 1:639:A:MET:HE1  | 7        | 2.94          |
| (1,596) | 1:632:A:ALA:HB3  | 1:635:A:VAL:HG21 | 20       | 2.94          |
| (1,480) | 1:653:A:LEU:HD21 | 1:636:A:GLU:HA   | 11       | 2.94          |
| (1,430) | 1:664:A:LEU:HD22 | 1:661:A:GLN:HA   | 9        | 2.94          |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG23 | 9        | 2.94          |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG21 | 14       | 2.94          |
| (1,129) | 1:652:A:LEU:HD21 | 1:649:A:TYR:HA   | 2        | 2.94          |
| (1,640) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD11 | 16       | 2.93          |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 8        | 2.93          |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 10       | 2.93          |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 15       | 2.93          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 1        | 2.92          |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 4        | 2.92          |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 1        | 2.92          |
| (1,559) | 1:603:A:LEU:HD22 | 1:600:A:ARG:HA   | 17       | 2.92          |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD21 | 13       | 2.91          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD12 | 16       | 2.91          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD12 | 16       | 2.91          |
| (1,480) | 1:653:A:LEU:HD23 | 1:636:A:GLU:HA   | 8        | 2.91          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 16       | 2.9           |
| (1,927) | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 5        | 2.9           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,927) | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 9        | 2.9           |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 6        | 2.9           |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 20       | 2.9           |
| (1,626) | 1:625:A:MET:HE2  | 1:628:A:LEU:HD13 | 8        | 2.9           |
| (1,480) | 1:653:A:LEU:HD23 | 1:636:A:GLU:HA   | 3        | 2.9           |
| (1,430) | 1:664:A:LEU:HD21 | 1:661:A:GLN:HA   | 10       | 2.9           |
| (1,605) | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD21 | 10       | 2.89          |
| (1,597) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD1  | 1        | 2.89          |
| (1,597) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD2  | 1        | 2.89          |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG23 | 4        | 2.89          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB1  | 20       | 2.89          |
| (1,129) | 1:652:A:LEU:HD21 | 1:649:A:TYR:HA   | 6        | 2.89          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE1  | 14       | 2.89          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE2  | 14       | 2.89          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD11 | 2        | 2.89          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD11 | 2        | 2.89          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD11 | 4        | 2.89          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD11 | 4        | 2.89          |
| (1,623) | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD11 | 13       | 2.88          |
| (1,601) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD1  | 17       | 2.88          |
| (1,601) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD2  | 17       | 2.88          |
| (1,524) | 1:595:A:VAL:HG23 | 1:646:A:ARG:HD3  | 14       | 2.88          |
| (1,430) | 1:664:A:LEU:HD23 | 1:661:A:GLN:HA   | 19       | 2.88          |
| (1,5)   | 1:608:A:VAL:HG21 | 1:625:A:MET:HE3  | 12       | 2.88          |
| (1,738) | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 14       | 2.87          |
| (1,659) | 1:652:A:LEU:HB3  | 1:639:A:MET:HE1  | 8        | 2.87          |
| (1,640) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD13 | 15       | 2.87          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD11 | 2        | 2.87          |
| (1,617) | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 15       | 2.87          |
| (1,559) | 1:603:A:LEU:HD21 | 1:600:A:ARG:HA   | 14       | 2.87          |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD21 | 16       | 2.87          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD13 | 20       | 2.87          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD13 | 20       | 2.87          |
| (1,20)  | 1:660:A:ILE:HG22 | 1:664:A:LEU:HD22 | 12       | 2.87          |
| (1,4)   | 1:629:A:VAL:HG22 | 1:625:A:MET:HE1  | 13       | 2.87          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 3        | 2.86          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 10       | 2.86          |
| (1,927) | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 18       | 2.86          |
| (1,626) | 1:625:A:MET:HE1  | 1:628:A:LEU:HD12 | 10       | 2.86          |
| (1,620) | 1:625:A:MET:HG2  | 1:620:A:LEU:HD13 | 6        | 2.86          |
| (1,601) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HD1  | 20       | 2.86          |
| (1,601) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HD2  | 20       | 2.86          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,535) | 1:639:A:MET:HG3  | 1:653:A:LEU:HD21 | 15       | 2.86          |
| (1,430) | 1:664:A:LEU:HD22 | 1:661:A:GLN:HA   | 16       | 2.86          |
| (1,20)  | 1:660:A:ILE:HG21 | 1:664:A:LEU:HD23 | 8        | 2.86          |
| (1,927) | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 15       | 2.85          |
| (1,679) | 1:643:A:ALA:H    | 1:652:A:LEU:HD23 | 18       | 2.85          |
| (1,659) | 1:652:A:LEU:HB3  | 1:639:A:MET:HE2  | 11       | 2.85          |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 18       | 2.85          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD13 | 18       | 2.85          |
| (1,596) | 1:632:A:ALA:HB1  | 1:635:A:VAL:HG22 | 11       | 2.85          |
| (1,5)   | 1:608:A:VAL:HG22 | 1:625:A:MET:HE1  | 18       | 2.85          |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 12       | 2.84          |
| (1,632) | 1:644:A:ASN:HD21 | 1:645:A:SER:HA   | 3        | 2.84          |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD23 | 16       | 2.84          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD11 | 11       | 2.84          |
| (1,601) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HD1  | 6        | 2.84          |
| (1,601) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HD2  | 6        | 2.84          |
| (1,376) | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 8        | 2.84          |
| (1,375) | 1:633:A:LYS:HD2  | 1:629:A:VAL:HG13 | 19       | 2.84          |
| (1,171) | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 16       | 2.84          |
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD12 | 12       | 2.83          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD13 | 5        | 2.83          |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD21 | 15       | 2.83          |
| (1,484) | 1:607:A:LEU:HD21 | 1:653:A:LEU:HB2  | 19       | 2.83          |
| (1,430) | 1:664:A:LEU:HD23 | 1:661:A:GLN:HA   | 2        | 2.83          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 17       | 2.83          |
| (1,226) | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG22 | 12       | 2.83          |
| (1,129) | 1:652:A:LEU:HD23 | 1:649:A:TYR:HA   | 9        | 2.83          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD13 | 3        | 2.83          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD13 | 3        | 2.83          |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 20       | 2.82          |
| (1,927) | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 7        | 2.82          |
| (1,659) | 1:652:A:LEU:HB3  | 1:639:A:MET:HE2  | 12       | 2.82          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD13 | 1        | 2.82          |
| (1,620) | 1:625:A:MET:HG2  | 1:620:A:LEU:HD12 | 18       | 2.82          |
| (1,617) | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 13       | 2.82          |
| (1,430) | 1:664:A:LEU:HD23 | 1:661:A:GLN:HA   | 15       | 2.82          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 19       | 2.81          |
| (1,738) | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 16       | 2.81          |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD21 | 19       | 2.81          |
| (1,626) | 1:625:A:MET:HE2  | 1:628:A:LEU:HD11 | 4        | 2.81          |
| (1,430) | 1:664:A:LEU:HD21 | 1:661:A:GLN:HA   | 13       | 2.81          |
| (1,376) | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG11 | 3        | 2.81          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,22)   | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE1  | 20       | 2.8           |
| (3,22)   | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE2  | 20       | 2.8           |
| (3,22)   | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE1  | 20       | 2.8           |
| (3,22)   | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE2  | 20       | 2.8           |
| (3,22)   | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE1  | 20       | 2.8           |
| (3,22)   | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE2  | 20       | 2.8           |
| (1,927)  | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 4        | 2.8           |
| (1,927)  | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 17       | 2.8           |
| (1,679)  | 1:643:A:ALA:H    | 1:652:A:LEU:HD23 | 9        | 2.8           |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD1  | 3        | 2.8           |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD2  | 3        | 2.8           |
| (1,596)  | 1:632:A:ALA:HB3  | 1:635:A:VAL:HG23 | 8        | 2.8           |
| (1,171)  | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 20       | 2.8           |
| (1,121)  | 1:653:A:LEU:HD12 | 1:649:A:TYR:HE1  | 18       | 2.8           |
| (1,121)  | 1:653:A:LEU:HD12 | 1:649:A:TYR:HE2  | 18       | 2.8           |
| (1,929)  | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 5        | 2.79          |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD12 | 8        | 2.79          |
| (1,605)  | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD22 | 9        | 2.79          |
| (1,603)  | 1:599:A:LEU:HD12 | 1:595:A:VAL:HG13 | 3        | 2.79          |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG23 | 5        | 2.79          |
| (1,129)  | 1:652:A:LEU:HD23 | 1:649:A:TYR:HA   | 3        | 2.79          |
| (1,129)  | 1:652:A:LEU:HD22 | 1:649:A:TYR:HA   | 5        | 2.79          |
| (1,129)  | 1:652:A:LEU:HD21 | 1:649:A:TYR:HA   | 20       | 2.79          |
| (1,20)   | 1:660:A:ILE:HG21 | 1:664:A:LEU:HD22 | 9        | 2.79          |
| (1,617)  | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 16       | 2.78          |
| (1,610)  | 1:599:A:LEU:HD21 | 1:603:A:LEU:HD21 | 13       | 2.78          |
| (1,596)  | 1:632:A:ALA:HB1  | 1:635:A:VAL:HG22 | 9        | 2.78          |
| (1,596)  | 1:632:A:ALA:HB3  | 1:635:A:VAL:HG22 | 17       | 2.78          |
| (1,430)  | 1:664:A:LEU:HD22 | 1:661:A:GLN:HA   | 1        | 2.78          |
| (1,248)  | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 1        | 2.78          |
| (1,226)  | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG22 | 11       | 2.78          |
| (1,171)  | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 11       | 2.78          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 10       | 2.77          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 10       | 2.77          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 10       | 2.77          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 10       | 2.77          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 10       | 2.77          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 10       | 2.77          |
| (1,927)  | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 16       | 2.77          |
| (1,679)  | 1:643:A:ALA:H    | 1:652:A:LEU:HD21 | 20       | 2.77          |
| (1,622)  | 1:608:A:VAL:HA   | 1:628:A:LEU:HD12 | 8        | 2.77          |
| (1,294)  | 1:604:A:VAL:HG13 | 1:633:A:LYS:HD2  | 10       | 2.77          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,626) | 1:625:A:MET:HE2  | 1:628:A:LEU:HD13 | 15       | 2.76          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD11 | 12       | 2.76          |
| (1,596) | 1:632:A:ALA:HB1  | 1:635:A:VAL:HG21 | 2        | 2.76          |
| (1,596) | 1:632:A:ALA:HB2  | 1:635:A:VAL:HG21 | 16       | 2.76          |
| (1,567) | 1:595:A:VAL:HA   | 1:594:A:HIS:HD2  | 18       | 2.76          |
| (1,435) | 1:653:A:LEU:HD12 | 1:639:A:MET:HE2  | 9        | 2.76          |
| (1,430) | 1:664:A:LEU:HD23 | 1:661:A:GLN:HA   | 20       | 2.76          |
| (1,376) | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG11 | 6        | 2.76          |
| (1,376) | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 17       | 2.76          |
| (1,294) | 1:604:A:VAL:HG13 | 1:633:A:LYS:HD2  | 18       | 2.76          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE1  | 4        | 2.76          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE2  | 4        | 2.76          |
| (1,20)  | 1:660:A:ILE:HG22 | 1:664:A:LEU:HD21 | 7        | 2.76          |
| (1,376) | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG13 | 15       | 2.75          |
| (1,171) | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 10       | 2.75          |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 18       | 2.75          |
| (1,121) | 1:653:A:LEU:HD12 | 1:649:A:TYR:HE1  | 13       | 2.75          |
| (1,121) | 1:653:A:LEU:HD12 | 1:649:A:TYR:HE2  | 13       | 2.75          |
| (1,679) | 1:643:A:ALA:H    | 1:652:A:LEU:HD23 | 1        | 2.74          |
| (1,477) | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG21 | 13       | 2.74          |
| (1,171) | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 8        | 2.74          |
| (1,171) | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 9        | 2.74          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD11 | 11       | 2.74          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD11 | 11       | 2.74          |
| (1,33)  | 1:652:A:LEU:HD21 | 1:643:A:ALA:HB1  | 2        | 2.74          |
| (1,927) | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 10       | 2.73          |
| (1,171) | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 3        | 2.73          |
| (1,171) | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 6        | 2.73          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE1  | 12       | 2.73          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE2  | 12       | 2.73          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD11 | 19       | 2.73          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD11 | 19       | 2.73          |
| (1,20)  | 1:660:A:ILE:HG22 | 1:664:A:LEU:HD22 | 1        | 2.73          |
| (1,961) | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 2        | 2.72          |
| (1,961) | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 9        | 2.72          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD11 | 17       | 2.72          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD1  | 8        | 2.72          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD2  | 8        | 2.72          |
| (1,524) | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD3  | 18       | 2.72          |
| (1,229) | 1:636:A:GLU:HG2  | 1:604:A:VAL:HG23 | 1        | 2.72          |
| (1,130) | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 11       | 2.72          |
| (1,129) | 1:652:A:LEU:HD23 | 1:649:A:TYR:HA   | 1        | 2.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,104)  | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 14       | 2.71          |
| (2,75)   | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 3        | 2.71          |
| (2,75)   | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 3        | 2.71          |
| (2,75)   | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 3        | 2.71          |
| (2,75)   | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 3        | 2.71          |
| (2,75)   | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 3        | 2.71          |
| (2,75)   | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 3        | 2.71          |
| (1,679)  | 1:643:A:ALA:H    | 1:652:A:LEU:HD23 | 17       | 2.71          |
| (1,659)  | 1:652:A:LEU:HB3  | 1:639:A:MET:HE3  | 2        | 2.71          |
| (1,629)  | 1:625:A:MET:HA   | 1:628:A:LEU:HD23 | 6        | 2.71          |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD22 | 7        | 2.71          |
| (2,104)  | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 9        | 2.7           |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 15       | 2.7           |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 15       | 2.7           |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 15       | 2.7           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 15       | 2.7           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 15       | 2.7           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 15       | 2.7           |
| (1,623)  | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD13 | 16       | 2.7           |
| (1,622)  | 1:608:A:VAL:HA   | 1:628:A:LEU:HD13 | 19       | 2.7           |
| (1,406)  | 1:635:A:VAL:HG22 | 1:656:A:LYS:HG2  | 15       | 2.7           |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 14       | 2.7           |
| (1,33)   | 1:652:A:LEU:HD23 | 1:643:A:ALA:HB3  | 18       | 2.7           |
| (1,559)  | 1:603:A:LEU:HD22 | 1:600:A:ARG:HA   | 11       | 2.69          |
| (1,226)  | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG22 | 16       | 2.69          |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 1        | 2.69          |
| (1,679)  | 1:643:A:ALA:H    | 1:652:A:LEU:HD23 | 3        | 2.68          |
| (1,523)  | 1:595:A:VAL:HG23 | 1:646:A:ARG:HD2  | 15       | 2.68          |
| (1,294)  | 1:604:A:VAL:HG11 | 1:633:A:LYS:HD2  | 6        | 2.68          |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 3        | 2.68          |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 12       | 2.68          |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 19       | 2.68          |
| (1,20)   | 1:660:A:ILE:HG22 | 1:664:A:LEU:HD22 | 4        | 2.68          |
| (1,20)   | 1:660:A:ILE:HG22 | 1:664:A:LEU:HD22 | 15       | 2.68          |
| (1,610)  | 1:599:A:LEU:HD22 | 1:603:A:LEU:HD22 | 10       | 2.67          |
| (1,523)  | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD2  | 18       | 2.67          |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD23 | 8        | 2.67          |
| (1,430)  | 1:664:A:LEU:HD22 | 1:661:A:GLN:HA   | 5        | 2.67          |
| (1,406)  | 1:635:A:VAL:HG23 | 1:656:A:LYS:HG2  | 6        | 2.67          |
| (1,219)  | 1:604:A:VAL:HA   | 1:607:A:LEU:HD22 | 4        | 2.67          |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 5        | 2.67          |
| (1,129)  | 1:652:A:LEU:HD21 | 1:649:A:TYR:HA   | 8        | 2.67          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,105)  | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 17       | 2.66          |
| (1,171)  | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 5        | 2.66          |
| (1,20)   | 1:660:A:ILE:HG21 | 1:664:A:LEU:HD21 | 11       | 2.66          |
| (1,6)    | 1:608:A:VAL:HG13 | 1:625:A:MET:HE3  | 1        | 2.66          |
| (1,961)  | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 16       | 2.65          |
| (1,627)  | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD21 | 19       | 2.65          |
| (1,559)  | 1:603:A:LEU:HD22 | 1:600:A:ARG:HA   | 18       | 2.65          |
| (1,480)  | 1:653:A:LEU:HD23 | 1:636:A:GLU:HA   | 2        | 2.65          |
| (1,359)  | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD23 | 16       | 2.65          |
| (1,219)  | 1:604:A:VAL:HA   | 1:607:A:LEU:HD21 | 5        | 2.65          |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 17       | 2.65          |
| (1,4)    | 1:629:A:VAL:HG23 | 1:625:A:MET:HE1  | 20       | 2.65          |
| (1,626)  | 1:625:A:MET:HE1  | 1:628:A:LEU:HD11 | 16       | 2.64          |
| (1,523)  | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD2  | 19       | 2.64          |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD23 | 20       | 2.64          |
| (1,487)  | 1:664:A:LEU:HD11 | 1:667:A:LYS:HG2  | 3        | 2.64          |
| (1,376)  | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 1        | 2.64          |
| (1,294)  | 1:604:A:VAL:HG11 | 1:633:A:LYS:HD2  | 15       | 2.64          |
| (1,171)  | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 18       | 2.64          |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 9        | 2.64          |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 13       | 2.64          |
| (1,119)  | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD13 | 14       | 2.64          |
| (1,119)  | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD13 | 14       | 2.64          |
| (1,24)   | 1:650:A:TYR:HA   | 1:653:A:LEU:HD13 | 12       | 2.64          |
| (1,547)  | 1:603:A:LEU:HD11 | 1:606:A:LYS:HD2  | 15       | 2.63          |
| (1,415)  | 1:620:A:LEU:HD21 | 1:625:A:MET:HG2  | 15       | 2.63          |
| (1,294)  | 1:604:A:VAL:HG12 | 1:633:A:LYS:HD2  | 8        | 2.63          |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 20       | 2.63          |
| (1,1)    | 1:656:A:LYS:HE2  | 1:639:A:MET:HE2  | 14       | 2.63          |
| (1,601)  | 1:595:A:VAL:HG12 | 1:640:A:TYR:HD1  | 15       | 2.62          |
| (1,601)  | 1:595:A:VAL:HG12 | 1:640:A:TYR:HD2  | 15       | 2.62          |
| (1,492)  | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 7        | 2.62          |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG22 | 16       | 2.62          |
| (1,467)  | 1:652:A:LEU:HD23 | 1:643:A:ALA:HA   | 11       | 2.62          |
| (1,129)  | 1:652:A:LEU:HD23 | 1:649:A:TYR:HA   | 7        | 2.62          |
| (1,33)   | 1:652:A:LEU:HD22 | 1:643:A:ALA:HB2  | 10       | 2.62          |
| (1,20)   | 1:660:A:ILE:HG23 | 1:664:A:LEU:HD22 | 5        | 2.62          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 5        | 2.61          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 5        | 2.61          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 5        | 2.61          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 5        | 2.61          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 5        | 2.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 5        | 2.61          |
| (1,626)  | 1:625:A:MET:HE2  | 1:628:A:LEU:HD11 | 14       | 2.61          |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG23 | 8        | 2.61          |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG23 | 15       | 2.61          |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 18       | 2.61          |
| (1,20)   | 1:660:A:ILE:HG21 | 1:664:A:LEU:HD22 | 16       | 2.61          |
| (1,4)    | 1:629:A:VAL:HG21 | 1:625:A:MET:HE3  | 12       | 2.61          |
| (1,594)  | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG13 | 20       | 2.6           |
| (1,492)  | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 20       | 2.6           |
| (1,484)  | 1:607:A:LEU:HD22 | 1:653:A:LEU:HB2  | 18       | 2.6           |
| (1,226)  | 1:633:A:LYS:HD2  | 1:604:A:VAL:HG22 | 5        | 2.6           |
| (1,171)  | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 4        | 2.6           |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 8        | 2.6           |
| (1,86)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 17       | 2.6           |
| (1,33)   | 1:652:A:LEU:HD23 | 1:643:A:ALA:HB2  | 9        | 2.6           |
| (1,679)  | 1:643:A:ALA:H    | 1:652:A:LEU:HD21 | 12       | 2.59          |
| (1,597)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HD1  | 9        | 2.59          |
| (1,597)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HD2  | 9        | 2.59          |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD1  | 17       | 2.59          |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD2  | 17       | 2.59          |
| (1,559)  | 1:603:A:LEU:HD22 | 1:600:A:ARG:HA   | 19       | 2.59          |
| (1,480)  | 1:653:A:LEU:HD22 | 1:636:A:GLU:HA   | 7        | 2.59          |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG23 | 6        | 2.59          |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG22 | 9        | 2.59          |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG22 | 10       | 2.59          |
| (1,219)  | 1:604:A:VAL:HA   | 1:607:A:LEU:HD21 | 6        | 2.59          |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 6        | 2.59          |
| (1,20)   | 1:660:A:ILE:HG21 | 1:664:A:LEU:HD22 | 6        | 2.59          |
| (2,104)  | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 8        | 2.58          |
| (1,659)  | 1:652:A:LEU:HB3  | 1:639:A:MET:HE2  | 17       | 2.58          |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD11 | 1        | 2.58          |
| (1,617)  | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 5        | 2.58          |
| (1,596)  | 1:632:A:ALA:HB2  | 1:635:A:VAL:HG21 | 7        | 2.58          |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG22 | 2        | 2.58          |
| (1,376)  | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 10       | 2.58          |
| (1,130)  | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 15       | 2.58          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 4        | 2.57          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 4        | 2.57          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 4        | 2.57          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 4        | 2.57          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 4        | 2.57          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 4        | 2.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,961)  | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 15       | 2.57          |
| (1,961)  | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 17       | 2.57          |
| (1,20)   | 1:660:A:ILE:HG22 | 1:664:A:LEU:HD22 | 14       | 2.57          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 1        | 2.56          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 1        | 2.56          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 1        | 2.56          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 1        | 2.56          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 1        | 2.56          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 1        | 2.56          |
| (1,927)  | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 1        | 2.56          |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD1  | 19       | 2.56          |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD2  | 19       | 2.56          |
| (1,535)  | 1:639:A:MET:HG3  | 1:653:A:LEU:HD22 | 5        | 2.56          |
| (1,163)  | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 14       | 2.56          |
| (1,148)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE1  | 1        | 2.56          |
| (1,148)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE2  | 1        | 2.56          |
| (1,524)  | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD3  | 16       | 2.55          |
| (1,359)  | 1:603:A:LEU:HD11 | 1:599:A:LEU:HD21 | 13       | 2.55          |
| (1,117)  | 1:653:A:LEU:HD21 | 1:650:A:TYR:HD1  | 6        | 2.55          |
| (1,117)  | 1:653:A:LEU:HD21 | 1:650:A:TYR:HD2  | 6        | 2.55          |
| (1,33)   | 1:652:A:LEU:HD23 | 1:643:A:ALA:HB1  | 14       | 2.55          |
| (1,626)  | 1:625:A:MET:HE2  | 1:628:A:LEU:HD12 | 9        | 2.54          |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD21 | 4        | 2.54          |
| (1,248)  | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 12       | 2.54          |
| (1,129)  | 1:652:A:LEU:HD23 | 1:649:A:TYR:HA   | 11       | 2.54          |
| (1,33)   | 1:652:A:LEU:HD21 | 1:643:A:ALA:HB2  | 6        | 2.54          |
| (1,603)  | 1:599:A:LEU:HD12 | 1:595:A:VAL:HG11 | 11       | 2.53          |
| (1,596)  | 1:632:A:ALA:HB1  | 1:635:A:VAL:HG21 | 6        | 2.53          |
| (1,594)  | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG11 | 7        | 2.53          |
| (1,534)  | 1:639:A:MET:HG2  | 1:653:A:LEU:HD21 | 10       | 2.53          |
| (1,482)  | 1:664:A:LEU:HD11 | 1:667:A:LYS:HD2  | 12       | 2.53          |
| (1,171)  | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 15       | 2.53          |
| (1,148)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE1  | 8        | 2.53          |
| (1,148)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE2  | 8        | 2.53          |
| (1,129)  | 1:652:A:LEU:HD22 | 1:649:A:TYR:HA   | 15       | 2.53          |
| (1,129)  | 1:652:A:LEU:HD21 | 1:649:A:TYR:HA   | 16       | 2.53          |
| (1,659)  | 1:652:A:LEU:HB3  | 1:639:A:MET:HE1  | 18       | 2.52          |
| (1,640)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD12 | 1        | 2.52          |
| (1,624)  | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD13 | 4        | 2.52          |
| (1,624)  | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD13 | 4        | 2.52          |
| (1,622)  | 1:608:A:VAL:HA   | 1:628:A:LEU:HD11 | 20       | 2.52          |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD11 | 5        | 2.52          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,596)  | 1:632:A:ALA:HB3  | 1:635:A:VAL:HG22 | 14       | 2.52          |
| (1,594)  | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG13 | 14       | 2.52          |
| (1,462)  | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 5        | 2.52          |
| (1,141)  | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE1  | 5        | 2.52          |
| (1,141)  | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE2  | 5        | 2.52          |
| (1,33)   | 1:652:A:LEU:HD23 | 1:643:A:ALA:HB1  | 1        | 2.52          |
| (1,629)  | 1:625:A:MET:HA   | 1:628:A:LEU:HD22 | 16       | 2.51          |
| (1,492)  | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 8        | 2.51          |
| (1,129)  | 1:652:A:LEU:HD22 | 1:649:A:TYR:HA   | 10       | 2.51          |
| (1,129)  | 1:652:A:LEU:HD22 | 1:649:A:TYR:HA   | 13       | 2.51          |
| (1,129)  | 1:652:A:LEU:HD23 | 1:649:A:TYR:HA   | 18       | 2.51          |
| (1,20)   | 1:660:A:ILE:HG22 | 1:664:A:LEU:HD23 | 20       | 2.51          |
| (1,961)  | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 3        | 2.5           |
| (1,927)  | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 14       | 2.5           |
| (1,535)  | 1:639:A:MET:HG3  | 1:653:A:LEU:HD22 | 4        | 2.5           |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD23 | 16       | 2.5           |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG21 | 17       | 2.5           |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG22 | 20       | 2.5           |
| (1,141)  | 1:595:A:VAL:HG23 | 1:640:A:TYR:HE1  | 1        | 2.5           |
| (1,141)  | 1:595:A:VAL:HG23 | 1:640:A:TYR:HE2  | 1        | 2.5           |
| (1,129)  | 1:652:A:LEU:HD23 | 1:649:A:TYR:HA   | 14       | 2.5           |
| (1,33)   | 1:652:A:LEU:HD23 | 1:643:A:ALA:HB3  | 3        | 2.5           |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 11       | 2.49          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 11       | 2.49          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 11       | 2.49          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 13       | 2.49          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 13       | 2.49          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 13       | 2.49          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 11       | 2.49          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 11       | 2.49          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 11       | 2.49          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 13       | 2.49          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 13       | 2.49          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 13       | 2.49          |
| (1,607)  | 1:599:A:LEU:HD21 | 1:602:A:HIS:HB2  | 19       | 2.49          |
| (1,596)  | 1:632:A:ALA:HB1  | 1:635:A:VAL:HG23 | 4        | 2.49          |
| (1,176)  | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB2  | 6        | 2.49          |
| (1,33)   | 1:652:A:LEU:HD21 | 1:643:A:ALA:HB1  | 19       | 2.49          |
| (1,622)  | 1:608:A:VAL:HA   | 1:628:A:LEU:HD11 | 7        | 2.48          |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD13 | 14       | 2.48          |
| (1,376)  | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 18       | 2.48          |
| (1,294)  | 1:604:A:VAL:HG13 | 1:633:A:LYS:HD2  | 17       | 2.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,163)  | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 12       | 2.48          |
| (1,86)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 2        | 2.48          |
| (1,86)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 10       | 2.48          |
| (1,659)  | 1:652:A:LEU:HB3  | 1:639:A:MET:HE3  | 19       | 2.47          |
| (1,603)  | 1:599:A:LEU:HD12 | 1:595:A:VAL:HG13 | 15       | 2.47          |
| (1,601)  | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD1  | 11       | 2.47          |
| (1,601)  | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD2  | 11       | 2.47          |
| (1,547)  | 1:603:A:LEU:HD13 | 1:606:A:LYS:HD2  | 4        | 2.47          |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG22 | 3        | 2.47          |
| (1,462)  | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 8        | 2.47          |
| (1,359)  | 1:603:A:LEU:HD11 | 1:599:A:LEU:HD22 | 10       | 2.47          |
| (1,348)  | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD11 | 5        | 2.47          |
| (1,86)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 18       | 2.47          |
| (1,33)   | 1:652:A:LEU:HD23 | 1:643:A:ALA:HB2  | 11       | 2.47          |
| (1,596)  | 1:632:A:ALA:HB2  | 1:635:A:VAL:HG22 | 13       | 2.46          |
| (1,523)  | 1:595:A:VAL:HG23 | 1:646:A:ARG:HD2  | 14       | 2.46          |
| (1,33)   | 1:652:A:LEU:HD21 | 1:643:A:ALA:HB2  | 12       | 2.46          |
| (1,4)    | 1:629:A:VAL:HG22 | 1:625:A:MET:HE2  | 7        | 2.46          |
| (1,607)  | 1:599:A:LEU:HD23 | 1:602:A:HIS:HB2  | 11       | 2.45          |
| (1,603)  | 1:599:A:LEU:HD13 | 1:595:A:VAL:HG12 | 6        | 2.45          |
| (1,39)   | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 2        | 2.45          |
| (1,640)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD12 | 19       | 2.44          |
| (1,596)  | 1:632:A:ALA:HB1  | 1:635:A:VAL:HG21 | 1        | 2.44          |
| (1,536)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD23 | 6        | 2.44          |
| (1,523)  | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD2  | 8        | 2.44          |
| (1,434)  | 1:635:A:VAL:HG22 | 1:639:A:MET:HE3  | 15       | 2.44          |
| (1,219)  | 1:604:A:VAL:HA   | 1:607:A:LEU:HD21 | 1        | 2.44          |
| (1,148)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HE1  | 6        | 2.44          |
| (1,148)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HE2  | 6        | 2.44          |
| (1,679)  | 1:643:A:ALA:H    | 1:652:A:LEU:HD22 | 15       | 2.43          |
| (1,659)  | 1:652:A:LEU:HB3  | 1:639:A:MET:HE2  | 3        | 2.43          |
| (1,536)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD23 | 4        | 2.43          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 9        | 2.42          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 9        | 2.42          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 9        | 2.42          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 9        | 2.42          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 9        | 2.42          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 9        | 2.42          |
| (1,629)  | 1:625:A:MET:HA   | 1:628:A:LEU:HD22 | 10       | 2.42          |
| (1,596)  | 1:632:A:ALA:HB2  | 1:635:A:VAL:HG22 | 3        | 2.42          |
| (1,594)  | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG11 | 1        | 2.42          |
| (1,480)  | 1:653:A:LEU:HD22 | 1:636:A:GLU:HA   | 5        | 2.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,87)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 5        | 2.42          |
| (1,86)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 19       | 2.42          |
| (1,480)  | 1:653:A:LEU:HD23 | 1:636:A:GLU:HA   | 4        | 2.41          |
| (1,430)  | 1:664:A:LEU:HD23 | 1:661:A:GLN:HA   | 7        | 2.41          |
| (1,20)   | 1:660:A:ILE:HG21 | 1:664:A:LEU:HD21 | 10       | 2.41          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 18       | 2.4           |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 18       | 2.4           |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 18       | 2.4           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 18       | 2.4           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 18       | 2.4           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 18       | 2.4           |
| (1,629)  | 1:625:A:MET:HA   | 1:628:A:LEU:HD21 | 14       | 2.4           |
| (1,467)  | 1:652:A:LEU:HD23 | 1:643:A:ALA:HA   | 1        | 2.4           |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD11 | 9        | 2.39          |
| (1,607)  | 1:599:A:LEU:HD21 | 1:602:A:HIS:HB2  | 4        | 2.39          |
| (1,467)  | 1:652:A:LEU:HD23 | 1:643:A:ALA:HA   | 14       | 2.39          |
| (1,87)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 14       | 2.39          |
| (1,87)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 15       | 2.39          |
| (1,33)   | 1:652:A:LEU:HD21 | 1:643:A:ALA:HB3  | 20       | 2.39          |
| (1,20)   | 1:660:A:ILE:HG21 | 1:664:A:LEU:HD21 | 17       | 2.39          |
| (1,641)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD12 | 19       | 2.38          |
| (1,623)  | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD11 | 9        | 2.38          |
| (1,535)  | 1:639:A:MET:HG3  | 1:653:A:LEU:HD22 | 17       | 2.38          |
| (1,496)  | 1:599:A:LEU:HD13 | 1:603:A:LEU:HD22 | 18       | 2.38          |
| (1,492)  | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 1        | 2.38          |
| (1,467)  | 1:652:A:LEU:HD22 | 1:643:A:ALA:HA   | 10       | 2.38          |
| (1,467)  | 1:652:A:LEU:HD23 | 1:643:A:ALA:HA   | 18       | 2.38          |
| (1,423)  | 1:629:A:VAL:HG12 | 1:626:A:GLU:HG2  | 8        | 2.38          |
| (1,961)  | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 13       | 2.37          |
| (1,623)  | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD12 | 8        | 2.37          |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD11 | 11       | 2.37          |
| (1,607)  | 1:599:A:LEU:HD23 | 1:602:A:HIS:HB2  | 7        | 2.37          |
| (1,607)  | 1:599:A:LEU:HD23 | 1:602:A:HIS:HB2  | 12       | 2.37          |
| (1,492)  | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 3        | 2.37          |
| (1,129)  | 1:652:A:LEU:HD21 | 1:649:A:TYR:HA   | 12       | 2.37          |
| (1,87)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 6        | 2.37          |
| (1,33)   | 1:652:A:LEU:HD22 | 1:643:A:ALA:HB2  | 5        | 2.37          |
| (3,28)   | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE1  | 10       | 2.36          |
| (3,28)   | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE2  | 10       | 2.36          |
| (3,28)   | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE1  | 10       | 2.36          |
| (3,28)   | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE2  | 10       | 2.36          |
| (3,28)   | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE1  | 10       | 2.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,28)   | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE2  | 10       | 2.36          |
| (1,679)  | 1:643:A:ALA:H    | 1:652:A:LEU:HD21 | 8        | 2.36          |
| (1,406)  | 1:635:A:VAL:HG23 | 1:656:A:LYS:HG2  | 19       | 2.36          |
| (1,87)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 16       | 2.36          |
| (1,961)  | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 4        | 2.35          |
| (1,659)  | 1:652:A:LEU:HB3  | 1:639:A:MET:HE3  | 16       | 2.35          |
| (1,492)  | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 11       | 2.35          |
| (1,477)  | 1:594:A:HIS:HD2  | 1:595:A:VAL:HG23 | 11       | 2.35          |
| (1,420)  | 1:635:A:VAL:HG12 | 1:634:A:LYS:HE2  | 12       | 2.35          |
| (1,659)  | 1:652:A:LEU:HB3  | 1:639:A:MET:HE3  | 20       | 2.34          |
| (1,607)  | 1:599:A:LEU:HD21 | 1:602:A:HIS:HB2  | 6        | 2.34          |
| (1,547)  | 1:603:A:LEU:HD13 | 1:606:A:LYS:HD2  | 5        | 2.34          |
| (1,492)  | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 2        | 2.34          |
| (1,348)  | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD11 | 4        | 2.34          |
| (1,171)  | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 12       | 2.34          |
| (1,129)  | 1:652:A:LEU:HD21 | 1:649:A:TYR:HA   | 19       | 2.34          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 9        | 2.33          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 9        | 2.33          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 9        | 2.33          |
| (1,524)  | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD3  | 10       | 2.33          |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD23 | 12       | 2.33          |
| (1,467)  | 1:652:A:LEU:HD21 | 1:643:A:ALA:HA   | 2        | 2.33          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 16       | 2.32          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 16       | 2.32          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 16       | 2.32          |
| (1,679)  | 1:643:A:ALA:H    | 1:652:A:LEU:HD22 | 13       | 2.32          |
| (1,623)  | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD11 | 14       | 2.32          |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD12 | 4        | 2.32          |
| (1,495)  | 1:653:A:LEU:HD13 | 1:603:A:LEU:HD12 | 15       | 2.32          |
| (1,406)  | 1:635:A:VAL:HG23 | 1:656:A:LYS:HG2  | 18       | 2.32          |
| (1,92)   | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 20       | 2.32          |
| (1,927)  | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 12       | 2.31          |
| (1,640)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD12 | 18       | 2.31          |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD1  | 7        | 2.31          |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD2  | 7        | 2.31          |
| (1,559)  | 1:603:A:LEU:HD22 | 1:600:A:ARG:HA   | 10       | 2.31          |
| (1,536)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD22 | 20       | 2.31          |
| (1,430)  | 1:664:A:LEU:HD21 | 1:661:A:GLN:HA   | 17       | 2.31          |
| (1,374)  | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG11 | 19       | 2.31          |
| (1,219)  | 1:604:A:VAL:HA   | 1:607:A:LEU:HD21 | 10       | 2.31          |
| (1,219)  | 1:604:A:VAL:HA   | 1:607:A:LEU:HD22 | 13       | 2.31          |
| (1,148)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HE1  | 16       | 2.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,148)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HE2  | 16       | 2.31          |
| (1,5)    | 1:608:A:VAL:HG23 | 1:625:A:MET:HE2  | 17       | 2.31          |
| (1,961)  | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 7        | 2.3           |
| (1,641)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD12 | 12       | 2.3           |
| (1,640)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD11 | 11       | 2.3           |
| (1,535)  | 1:639:A:MET:HG3  | 1:653:A:LEU:HD21 | 16       | 2.3           |
| (1,496)  | 1:599:A:LEU:HD13 | 1:603:A:LEU:HD22 | 1        | 2.3           |
| (1,467)  | 1:652:A:LEU:HD21 | 1:643:A:ALA:HA   | 20       | 2.3           |
| (1,433)  | 1:656:A:LYS:HG2  | 1:639:A:MET:HE1  | 6        | 2.3           |
| (1,129)  | 1:652:A:LEU:HD22 | 1:649:A:TYR:HA   | 4        | 2.3           |
| (1,5)    | 1:608:A:VAL:HG22 | 1:625:A:MET:HE3  | 11       | 2.3           |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD22 | 11       | 2.29          |
| (1,467)  | 1:652:A:LEU:HD23 | 1:643:A:ALA:HA   | 9        | 2.29          |
| (1,430)  | 1:664:A:LEU:HD22 | 1:661:A:GLN:HA   | 3        | 2.29          |
| (1,142)  | 1:595:A:VAL:HG12 | 1:640:A:TYR:HE1  | 5        | 2.29          |
| (1,142)  | 1:595:A:VAL:HG12 | 1:640:A:TYR:HE2  | 5        | 2.29          |
| (1,33)   | 1:652:A:LEU:HD23 | 1:643:A:ALA:HB2  | 17       | 2.29          |
| (1,738)  | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 5        | 2.28          |
| (1,679)  | 1:643:A:ALA:H    | 1:652:A:LEU:HD23 | 7        | 2.28          |
| (1,623)  | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD13 | 19       | 2.28          |
| (1,492)  | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 18       | 2.28          |
| (1,141)  | 1:595:A:VAL:HG23 | 1:640:A:TYR:HE1  | 19       | 2.28          |
| (1,141)  | 1:595:A:VAL:HG23 | 1:640:A:TYR:HE2  | 19       | 2.28          |
| (1,33)   | 1:652:A:LEU:HD23 | 1:643:A:ALA:HB3  | 7        | 2.28          |
| (1,927)  | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 19       | 2.27          |
| (1,738)  | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 1        | 2.27          |
| (1,679)  | 1:643:A:ALA:H    | 1:652:A:LEU:HD21 | 19       | 2.27          |
| (1,607)  | 1:599:A:LEU:HD21 | 1:602:A:HIS:HB2  | 8        | 2.27          |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD22 | 14       | 2.27          |
| (1,467)  | 1:652:A:LEU:HD21 | 1:643:A:ALA:HA   | 6        | 2.27          |
| (1,467)  | 1:652:A:LEU:HD21 | 1:643:A:ALA:HA   | 8        | 2.27          |
| (1,294)  | 1:604:A:VAL:HG12 | 1:633:A:LYS:HD2  | 3        | 2.27          |
| (1,33)   | 1:652:A:LEU:HD21 | 1:643:A:ALA:HB3  | 8        | 2.27          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 8        | 2.26          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 8        | 2.26          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 8        | 2.26          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 8        | 2.26          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 8        | 2.26          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 8        | 2.26          |
| (1,20)   | 1:660:A:ILE:HG22 | 1:664:A:LEU:HD21 | 2        | 2.26          |
| (1,6)    | 1:608:A:VAL:HG13 | 1:625:A:MET:HE1  | 13       | 2.26          |
| (1,607)  | 1:599:A:LEU:HD21 | 1:602:A:HIS:HB2  | 20       | 2.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,524)  | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD3  | 20       | 2.25          |
| (1,423)  | 1:629:A:VAL:HG11 | 1:626:A:GLU:HG2  | 11       | 2.25          |
| (1,129)  | 1:652:A:LEU:HD23 | 1:649:A:TYR:HA   | 17       | 2.25          |
| (1,33)   | 1:652:A:LEU:HD22 | 1:643:A:ALA:HB3  | 13       | 2.25          |
| (1,20)   | 1:660:A:ILE:HG21 | 1:664:A:LEU:HD21 | 13       | 2.25          |
| (1,659)  | 1:652:A:LEU:HB3  | 1:639:A:MET:HE2  | 4        | 2.24          |
| (1,536)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD21 | 18       | 2.24          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 11       | 2.23          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 11       | 2.23          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 11       | 2.23          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 12       | 2.23          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 12       | 2.23          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 12       | 2.23          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 12       | 2.23          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 12       | 2.23          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 12       | 2.23          |
| (1,679)  | 1:643:A:ALA:H    | 1:652:A:LEU:HD21 | 16       | 2.23          |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD12 | 2        | 2.23          |
| (1,617)  | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 1        | 2.23          |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD23 | 2        | 2.23          |
| (1,467)  | 1:652:A:LEU:HD22 | 1:643:A:ALA:HA   | 15       | 2.23          |
| (1,436)  | 1:653:A:LEU:HA   | 1:639:A:MET:HE1  | 6        | 2.23          |
| (1,376)  | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 5        | 2.23          |
| (1,117)  | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD1  | 9        | 2.23          |
| (1,117)  | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD2  | 9        | 2.23          |
| (1,641)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD11 | 4        | 2.22          |
| (1,498)  | 1:639:A:MET:HG2  | 1:652:A:LEU:HD23 | 6        | 2.22          |
| (1,434)  | 1:635:A:VAL:HG21 | 1:639:A:MET:HE3  | 12       | 2.22          |
| (1,176)  | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB3  | 11       | 2.22          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 20       | 2.21          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 20       | 2.21          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 20       | 2.21          |
| (1,596)  | 1:632:A:ALA:HB2  | 1:635:A:VAL:HG23 | 15       | 2.21          |
| (1,547)  | 1:603:A:LEU:HD11 | 1:606:A:LYS:HD2  | 11       | 2.21          |
| (1,467)  | 1:652:A:LEU:HD21 | 1:643:A:ALA:HA   | 12       | 2.21          |
| (1,148)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HE1  | 9        | 2.21          |
| (1,148)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HE2  | 9        | 2.21          |
| (2,104)  | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 17       | 2.2           |
| (1,738)  | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 7        | 2.2           |
| (1,623)  | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD13 | 4        | 2.2           |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD13 | 20       | 2.2           |
| (1,607)  | 1:599:A:LEU:HD23 | 1:602:A:HIS:HB2  | 2        | 2.2           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,523) | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD2  | 17       | 2.2           |
| (1,467) | 1:652:A:LEU:HD21 | 1:643:A:ALA:HA   | 19       | 2.2           |
| (1,376) | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 11       | 2.2           |
| (1,219) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD23 | 19       | 2.2           |
| (1,961) | 1:588:A:ARG:H    | 1:589:A:LYS:HD2  | 12       | 2.19          |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD22 | 15       | 2.19          |
| (1,617) | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 18       | 2.19          |
| (1,492) | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 19       | 2.19          |
| (1,467) | 1:652:A:LEU:HD23 | 1:643:A:ALA:HA   | 3        | 2.19          |
| (1,467) | 1:652:A:LEU:HD23 | 1:643:A:ALA:HA   | 17       | 2.19          |
| (1,559) | 1:603:A:LEU:HD23 | 1:600:A:ARG:HA   | 20       | 2.18          |
| (1,499) | 1:639:A:MET:HG3  | 1:652:A:LEU:HD22 | 17       | 2.18          |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD22 | 9        | 2.18          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 15       | 2.18          |
| (1,148) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE1  | 4        | 2.18          |
| (1,148) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE2  | 4        | 2.18          |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE1  | 17       | 2.18          |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE2  | 17       | 2.18          |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD12 | 17       | 2.18          |
| (1,659) | 1:652:A:LEU:HB3  | 1:639:A:MET:HE1  | 1        | 2.17          |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD22 | 14       | 2.17          |
| (1,620) | 1:625:A:MET:HG2  | 1:620:A:LEU:HD12 | 3        | 2.17          |
| (1,597) | 1:635:A:VAL:HG11 | 1:631:A:TYR:HD1  | 6        | 2.17          |
| (1,597) | 1:635:A:VAL:HG11 | 1:631:A:TYR:HD2  | 6        | 2.17          |
| (1,559) | 1:603:A:LEU:HD21 | 1:600:A:ARG:HA   | 1        | 2.17          |
| (1,523) | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD2  | 1        | 2.17          |
| (1,499) | 1:639:A:MET:HG3  | 1:652:A:LEU:HD21 | 13       | 2.17          |
| (1,467) | 1:652:A:LEU:HD21 | 1:643:A:ALA:HA   | 16       | 2.17          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 20       | 2.17          |
| (1,376) | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 2        | 2.17          |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE1  | 3        | 2.17          |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE2  | 3        | 2.17          |
| (1,33)  | 1:652:A:LEU:HD22 | 1:643:A:ALA:HB1  | 15       | 2.17          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 17       | 2.16          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 17       | 2.16          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 17       | 2.16          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 17       | 2.16          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 17       | 2.16          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 17       | 2.16          |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD23 | 17       | 2.16          |
| (1,620) | 1:625:A:MET:HG2  | 1:620:A:LEU:HD11 | 12       | 2.15          |
| (1,620) | 1:625:A:MET:HG2  | 1:620:A:LEU:HD11 | 17       | 2.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,603)  | 1:599:A:LEU:HD12 | 1:595:A:VAL:HG12 | 19       | 2.15          |
| (1,495)  | 1:653:A:LEU:HD11 | 1:603:A:LEU:HD13 | 16       | 2.15          |
| (1,369)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD21 | 14       | 2.15          |
| (1,348)  | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD13 | 12       | 2.15          |
| (1,294)  | 1:604:A:VAL:HG12 | 1:633:A:LYS:HD2  | 13       | 2.15          |
| (1,171)  | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 1        | 2.15          |
| (1,33)   | 1:652:A:LEU:HD21 | 1:643:A:ALA:HB1  | 16       | 2.15          |
| (1,738)  | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 6        | 2.14          |
| (1,535)  | 1:639:A:MET:HG3  | 1:653:A:LEU:HD22 | 13       | 2.14          |
| (1,219)  | 1:604:A:VAL:HA   | 1:607:A:LEU:HD21 | 18       | 2.14          |
| (1,623)  | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD12 | 18       | 2.13          |
| (1,436)  | 1:653:A:LEU:HA   | 1:639:A:MET:HE2  | 9        | 2.13          |
| (1,376)  | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 9        | 2.13          |
| (1,5)    | 1:608:A:VAL:HG21 | 1:625:A:MET:HE3  | 8        | 2.13          |
| (1,617)  | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 20       | 2.12          |
| (1,600)  | 1:646:A:ARG:HA   | 1:595:A:VAL:HG22 | 6        | 2.12          |
| (1,597)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD1  | 10       | 2.12          |
| (1,597)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD2  | 10       | 2.12          |
| (1,406)  | 1:635:A:VAL:HG23 | 1:656:A:LYS:HG2  | 12       | 2.12          |
| (1,376)  | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG11 | 4        | 2.12          |
| (1,376)  | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG13 | 16       | 2.12          |
| (1,376)  | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG11 | 20       | 2.12          |
| (1,369)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD21 | 18       | 2.12          |
| (2,105)  | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 6        | 2.11          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 2        | 2.11          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 2        | 2.11          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 2        | 2.11          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 2        | 2.11          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 2        | 2.11          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 2        | 2.11          |
| (1,627)  | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD22 | 7        | 2.11          |
| (1,623)  | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD11 | 12       | 2.11          |
| (1,623)  | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD13 | 17       | 2.11          |
| (1,600)  | 1:646:A:ARG:HA   | 1:595:A:VAL:HG21 | 2        | 2.11          |
| (1,547)  | 1:603:A:LEU:HD12 | 1:606:A:LYS:HD2  | 17       | 2.11          |
| (1,523)  | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD2  | 2        | 2.11          |
| (1,376)  | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 14       | 2.11          |
| (1,603)  | 1:599:A:LEU:HD11 | 1:595:A:VAL:HG11 | 12       | 2.1           |
| (1,600)  | 1:646:A:ARG:HA   | 1:595:A:VAL:HG22 | 11       | 2.1           |
| (1,559)  | 1:603:A:LEU:HD21 | 1:600:A:ARG:HA   | 2        | 2.1           |
| (1,559)  | 1:603:A:LEU:HD21 | 1:600:A:ARG:HA   | 6        | 2.1           |
| (1,547)  | 1:603:A:LEU:HD13 | 1:606:A:LYS:HD2  | 18       | 2.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,534)  | 1:639:A:MET:HG2  | 1:653:A:LEU:HD22 | 4        | 2.1           |
| (1,484)  | 1:607:A:LEU:HD22 | 1:653:A:LEU:HB2  | 14       | 2.1           |
| (1,433)  | 1:656:A:LYS:HG2  | 1:639:A:MET:HE3  | 13       | 2.1           |
| (1,369)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD21 | 12       | 2.1           |
| (1,993)  | 1:619:A:ALA:HB1  | 1:612:A:PHE:HZ   | 7        | 2.09          |
| (1,993)  | 1:619:A:ALA:HB2  | 1:612:A:PHE:HZ   | 7        | 2.09          |
| (1,993)  | 1:619:A:ALA:HB3  | 1:612:A:PHE:HZ   | 7        | 2.09          |
| (1,467)  | 1:652:A:LEU:HD22 | 1:643:A:ALA:HA   | 13       | 2.09          |
| (1,348)  | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD12 | 15       | 2.09          |
| (3,22)   | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE1  | 2        | 2.08          |
| (3,22)   | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE2  | 2        | 2.08          |
| (3,22)   | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE1  | 2        | 2.08          |
| (3,22)   | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE2  | 2        | 2.08          |
| (3,22)   | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE1  | 2        | 2.08          |
| (3,22)   | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE2  | 2        | 2.08          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 20       | 2.08          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 20       | 2.08          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 20       | 2.08          |
| (1,738)  | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 3        | 2.08          |
| (1,641)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD13 | 6        | 2.08          |
| (1,617)  | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 7        | 2.08          |
| (1,610)  | 1:599:A:LEU:HD21 | 1:603:A:LEU:HD22 | 1        | 2.08          |
| (1,597)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD1  | 4        | 2.08          |
| (1,597)  | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD2  | 4        | 2.08          |
| (1,536)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD23 | 3        | 2.08          |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD23 | 6        | 2.08          |
| (1,20)   | 1:660:A:ILE:HG22 | 1:664:A:LEU:HD21 | 3        | 2.08          |
| (1,679)  | 1:643:A:ALA:H    | 1:652:A:LEU:HD22 | 5        | 2.07          |
| (1,640)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD13 | 8        | 2.07          |
| (1,620)  | 1:625:A:MET:HG2  | 1:620:A:LEU:HD11 | 19       | 2.07          |
| (1,594)  | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG12 | 6        | 2.07          |
| (1,523)  | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD2  | 3        | 2.07          |
| (1,434)  | 1:635:A:VAL:HG21 | 1:639:A:MET:HE1  | 19       | 2.07          |
| (1,366)  | 1:639:A:MET:HE3  | 1:653:A:LEU:HD23 | 1        | 2.07          |
| (1,4)    | 1:629:A:VAL:HG22 | 1:625:A:MET:HE3  | 11       | 2.07          |
| (1,679)  | 1:643:A:ALA:H    | 1:652:A:LEU:HD22 | 4        | 2.06          |
| (1,641)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD11 | 7        | 2.06          |
| (1,600)  | 1:646:A:ARG:HA   | 1:595:A:VAL:HG21 | 20       | 2.06          |
| (1,417)  | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD13 | 5        | 2.06          |
| (1,176)  | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB1  | 9        | 2.06          |
| (1,142)  | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE1  | 1        | 2.06          |
| (1,142)  | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE2  | 1        | 2.06          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,738) | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 9        | 2.05          |
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD13 | 8        | 2.05          |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD21 | 10       | 2.05          |
| (1,499) | 1:639:A:MET:HG3  | 1:652:A:LEU:HD22 | 3        | 2.05          |
| (1,438) | 1:672:A:LEU:HD13 | 1:671:A:ARG:HG3  | 8        | 2.05          |
| (1,434) | 1:635:A:VAL:HG22 | 1:639:A:MET:HE1  | 6        | 2.05          |
| (1,394) | 1:635:A:VAL:HG13 | 1:632:A:ALA:HA   | 11       | 2.05          |
| (1,394) | 1:635:A:VAL:HG11 | 1:632:A:ALA:HA   | 16       | 2.05          |
| (1,376) | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG13 | 7        | 2.05          |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD22 | 5        | 2.05          |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD12 | 9        | 2.05          |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE1  | 14       | 2.05          |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE2  | 14       | 2.05          |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD11 | 19       | 2.05          |
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD11 | 5        | 2.04          |
| (1,623) | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD11 | 20       | 2.04          |
| (1,603) | 1:599:A:LEU:HD13 | 1:595:A:VAL:HG12 | 8        | 2.04          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE1  | 7        | 2.04          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE2  | 7        | 2.04          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE1  | 20       | 2.04          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE2  | 20       | 2.04          |
| (1,738) | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 2        | 2.03          |
| (1,559) | 1:603:A:LEU:HD22 | 1:600:A:ARG:HA   | 7        | 2.03          |
| (1,496) | 1:599:A:LEU:HD12 | 1:603:A:LEU:HD22 | 16       | 2.03          |
| (1,467) | 1:652:A:LEU:HD23 | 1:643:A:ALA:HA   | 7        | 2.03          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD13 | 10       | 2.03          |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD13 | 2        | 2.03          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 10       | 2.02          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 10       | 2.02          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 10       | 2.02          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 10       | 2.02          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 10       | 2.02          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 10       | 2.02          |
| (1,623) | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD12 | 15       | 2.02          |
| (1,607) | 1:599:A:LEU:HD21 | 1:602:A:HIS:HB2  | 15       | 2.02          |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG22 | 14       | 2.02          |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG23 | 19       | 2.02          |
| (1,523) | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD2  | 10       | 2.02          |
| (1,467) | 1:652:A:LEU:HD22 | 1:643:A:ALA:HA   | 5        | 2.02          |
| (1,376) | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 13       | 2.02          |
| (1,318) | 1:652:A:LEU:HA   | 1:652:A:LEU:HD13 | 5        | 2.02          |
| (1,318) | 1:652:A:LEU:HA   | 1:652:A:LEU:HD12 | 16       | 2.02          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,303)  | 1:664:A:LEU:HD13 | 1:664:A:LEU:HA   | 7        | 2.02          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 17       | 2.01          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 17       | 2.01          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 17       | 2.01          |
| (1,617)  | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 11       | 2.01          |
| (1,559)  | 1:603:A:LEU:HD21 | 1:600:A:ARG:HA   | 15       | 2.01          |
| (1,523)  | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD2  | 20       | 2.01          |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD21 | 15       | 2.01          |
| (1,492)  | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 17       | 2.01          |
| (1,432)  | 1:653:A:LEU:HG   | 1:639:A:MET:HE1  | 3        | 2.01          |
| (1,369)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD22 | 5        | 2.01          |
| (1,348)  | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD13 | 8        | 2.01          |
| (1,318)  | 1:652:A:LEU:HA   | 1:652:A:LEU:HD12 | 4        | 2.01          |
| (1,303)  | 1:664:A:LEU:HD11 | 1:664:A:LEU:HA   | 6        | 2.01          |
| (1,303)  | 1:664:A:LEU:HD11 | 1:664:A:LEU:HA   | 18       | 2.01          |
| (1,39)   | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 7        | 2.01          |
| (1,4)    | 1:629:A:VAL:HG23 | 1:625:A:MET:HE3  | 8        | 2.01          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 17       | 2.0           |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 17       | 2.0           |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 17       | 2.0           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 17       | 2.0           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 17       | 2.0           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 17       | 2.0           |
| (1,610)  | 1:599:A:LEU:HD21 | 1:603:A:LEU:HD21 | 14       | 2.0           |
| (1,573)  | 1:657:A:ILE:HD12 | 1:606:A:LYS:HG2  | 5        | 2.0           |
| (1,318)  | 1:652:A:LEU:HA   | 1:652:A:LEU:HD12 | 8        | 2.0           |
| (2,168)  | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 14       | 1.99          |
| (1,603)  | 1:599:A:LEU:HD12 | 1:595:A:VAL:HG13 | 20       | 1.99          |
| (1,594)  | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG11 | 11       | 1.99          |
| (1,436)  | 1:653:A:LEU:HA   | 1:639:A:MET:HE1  | 3        | 1.99          |
| (1,406)  | 1:635:A:VAL:HG23 | 1:656:A:LYS:HG2  | 5        | 1.99          |
| (1,303)  | 1:664:A:LEU:HD11 | 1:664:A:LEU:HA   | 5        | 1.99          |
| (1,303)  | 1:664:A:LEU:HD11 | 1:664:A:LEU:HA   | 19       | 1.99          |
| (1,243)  | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 8        | 1.99          |
| (1,243)  | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 15       | 1.99          |
| (2,75)   | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 4        | 1.98          |
| (2,75)   | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 4        | 1.98          |
| (2,75)   | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 4        | 1.98          |
| (2,75)   | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 4        | 1.98          |
| (2,75)   | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 4        | 1.98          |
| (2,75)   | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 4        | 1.98          |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD22 | 9        | 1.98          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE1  | 6        | 1.98          |
| (1,359) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD21 | 14       | 1.98          |
| (1,318) | 1:652:A:LEU:HA   | 1:652:A:LEU:HD12 | 12       | 1.98          |
| (1,318) | 1:652:A:LEU:HA   | 1:652:A:LEU:HD13 | 13       | 1.98          |
| (1,318) | 1:652:A:LEU:HA   | 1:652:A:LEU:HD11 | 15       | 1.98          |
| (1,318) | 1:652:A:LEU:HA   | 1:652:A:LEU:HD12 | 19       | 1.98          |
| (1,303) | 1:664:A:LEU:HD11 | 1:664:A:LEU:HA   | 9        | 1.98          |
| (1,303) | 1:664:A:LEU:HD12 | 1:664:A:LEU:HA   | 16       | 1.98          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 8        | 1.98          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD1  | 8        | 1.97          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD2  | 8        | 1.97          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD1  | 8        | 1.97          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD2  | 8        | 1.97          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD1  | 8        | 1.97          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD2  | 8        | 1.97          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD1  | 9        | 1.97          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD2  | 9        | 1.97          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD1  | 9        | 1.97          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD2  | 9        | 1.97          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD1  | 9        | 1.97          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD2  | 9        | 1.97          |
| (1,607) | 1:599:A:LEU:HD21 | 1:602:A:HIS:HB2  | 3        | 1.97          |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG22 | 15       | 1.97          |
| (1,559) | 1:603:A:LEU:HD21 | 1:600:A:ARG:HA   | 3        | 1.97          |
| (1,433) | 1:656:A:LYS:HG2  | 1:639:A:MET:HE1  | 15       | 1.97          |
| (1,303) | 1:664:A:LEU:HD13 | 1:664:A:LEU:HA   | 1        | 1.97          |
| (1,303) | 1:664:A:LEU:HD13 | 1:664:A:LEU:HA   | 10       | 1.97          |
| (1,303) | 1:664:A:LEU:HD11 | 1:664:A:LEU:HA   | 12       | 1.97          |
| (1,303) | 1:664:A:LEU:HD11 | 1:664:A:LEU:HA   | 13       | 1.97          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 20       | 1.97          |
| (1,738) | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 19       | 1.96          |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD23 | 20       | 1.96          |
| (1,623) | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD11 | 11       | 1.96          |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG23 | 18       | 1.96          |
| (1,433) | 1:656:A:LYS:HG2  | 1:639:A:MET:HE2  | 5        | 1.96          |
| (1,318) | 1:652:A:LEU:HA   | 1:652:A:LEU:HD12 | 7        | 1.96          |
| (1,303) | 1:664:A:LEU:HD13 | 1:664:A:LEU:HA   | 14       | 1.96          |
| (1,294) | 1:604:A:VAL:HG12 | 1:633:A:LYS:HD2  | 2        | 1.96          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 5        | 1.96          |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE1  | 19       | 1.96          |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE2  | 19       | 1.96          |
| (1,116) | 1:653:A:LEU:HD12 | 1:650:A:TYR:HD1  | 17       | 1.96          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,116) | 1:653:A:LEU:HD12 | 1:650:A:TYR:HD2  | 17       | 1.96          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD1  | 5        | 1.95          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD2  | 5        | 1.95          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD1  | 5        | 1.95          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD2  | 5        | 1.95          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD1  | 5        | 1.95          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD2  | 5        | 1.95          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE1  | 14       | 1.95          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE2  | 14       | 1.95          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE1  | 14       | 1.95          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE2  | 14       | 1.95          |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE1  | 14       | 1.95          |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE2  | 14       | 1.95          |
| (1,499) | 1:639:A:MET:HG3  | 1:652:A:LEU:HD21 | 10       | 1.95          |
| (1,423) | 1:629:A:VAL:HG12 | 1:626:A:GLU:HG2  | 15       | 1.95          |
| (1,380) | 1:620:A:LEU:HD12 | 1:617:A:PRO:HA   | 15       | 1.95          |
| (1,318) | 1:652:A:LEU:HA   | 1:652:A:LEU:HD13 | 6        | 1.95          |
| (1,263) | 1:607:A:LEU:HD21 | 1:632:A:ALA:HB1  | 6        | 1.95          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 1        | 1.95          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 20       | 1.95          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE1  | 11       | 1.95          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE2  | 11       | 1.95          |
| (1,33)  | 1:652:A:LEU:HD22 | 1:643:A:ALA:HB3  | 4        | 1.95          |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD11 | 11       | 1.95          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD1  | 18       | 1.94          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD2  | 18       | 1.94          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD1  | 18       | 1.94          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD2  | 18       | 1.94          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD1  | 18       | 1.94          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD2  | 18       | 1.94          |
| (1,738) | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 8        | 1.94          |
| (1,640) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD11 | 7        | 1.94          |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD21 | 20       | 1.94          |
| (1,617) | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 19       | 1.94          |
| (1,603) | 1:599:A:LEU:HD11 | 1:595:A:VAL:HG11 | 7        | 1.94          |
| (1,559) | 1:603:A:LEU:HD22 | 1:600:A:ARG:HA   | 16       | 1.94          |
| (1,495) | 1:653:A:LEU:HD13 | 1:603:A:LEU:HD12 | 12       | 1.94          |
| (1,423) | 1:629:A:VAL:HG11 | 1:626:A:GLU:HG2  | 3        | 1.94          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD13 | 13       | 1.94          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB1  | 12       | 1.94          |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD21 | 15       | 1.94          |
| (1,303) | 1:664:A:LEU:HD11 | 1:664:A:LEU:HA   | 8        | 1.94          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,303) | 1:664:A:LEU:HD13 | 1:664:A:LEU:HA   | 20       | 1.94          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 14       | 1.94          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE1  | 8        | 1.94          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE2  | 8        | 1.94          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 13       | 1.94          |
| (1,4)   | 1:629:A:VAL:HG21 | 1:625:A:MET:HE3  | 15       | 1.94          |
| (1,738) | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 10       | 1.93          |
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD12 | 11       | 1.93          |
| (1,623) | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD12 | 1        | 1.93          |
| (1,622) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD13 | 3        | 1.93          |
| (1,229) | 1:636:A:GLU:HG2  | 1:604:A:VAL:HG23 | 20       | 1.93          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 3        | 1.92          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 2        | 1.92          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 2        | 1.92          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 2        | 1.92          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 2        | 1.92          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 2        | 1.92          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 2        | 1.92          |
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD13 | 2        | 1.92          |
| (1,640) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD13 | 20       | 1.92          |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD21 | 13       | 1.92          |
| (1,559) | 1:603:A:LEU:HD23 | 1:600:A:ARG:HA   | 13       | 1.92          |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD12 | 7        | 1.92          |
| (1,318) | 1:652:A:LEU:HA   | 1:652:A:LEU:HD12 | 18       | 1.92          |
| (1,303) | 1:664:A:LEU:HD11 | 1:664:A:LEU:HA   | 4        | 1.92          |
| (1,303) | 1:664:A:LEU:HD11 | 1:664:A:LEU:HA   | 17       | 1.92          |
| (1,141) | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE1  | 14       | 1.92          |
| (1,141) | 1:595:A:VAL:HG22 | 1:640:A:TYR:HE2  | 14       | 1.92          |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD1  | 7        | 1.92          |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD2  | 7        | 1.92          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 18       | 1.92          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB3  | 2        | 1.92          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 13       | 1.91          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 13       | 1.91          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 13       | 1.91          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 13       | 1.91          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 13       | 1.91          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 13       | 1.91          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 13       | 1.91          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 13       | 1.91          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 13       | 1.91          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 12       | 1.91          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,75)   | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 12       | 1.91          |
| (2,75)   | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 12       | 1.91          |
| (2,75)   | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 12       | 1.91          |
| (2,75)   | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 12       | 1.91          |
| (2,75)   | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 12       | 1.91          |
| (1,638)  | 1:639:A:MET:HA   | 1:652:A:LEU:HD23 | 6        | 1.91          |
| (1,638)  | 1:639:A:MET:HA   | 1:652:A:LEU:HD23 | 12       | 1.91          |
| (1,617)  | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 8        | 1.91          |
| (1,559)  | 1:603:A:LEU:HD22 | 1:600:A:ARG:HA   | 4        | 1.91          |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD23 | 19       | 1.91          |
| (1,406)  | 1:635:A:VAL:HG21 | 1:656:A:LYS:HG2  | 11       | 1.91          |
| (1,394)  | 1:635:A:VAL:HG11 | 1:632:A:ALA:HA   | 9        | 1.91          |
| (1,376)  | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 12       | 1.91          |
| (1,345)  | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD12 | 18       | 1.91          |
| (1,318)  | 1:652:A:LEU:HA   | 1:652:A:LEU:HD13 | 1        | 1.91          |
| (1,278)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 2        | 1.91          |
| (1,278)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 11       | 1.91          |
| (1,278)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 16       | 1.91          |
| (1,243)  | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 17       | 1.91          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 12       | 1.9           |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 12       | 1.9           |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 12       | 1.9           |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 20       | 1.9           |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 20       | 1.9           |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 20       | 1.9           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 20       | 1.9           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 20       | 1.9           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 20       | 1.9           |
| (1,738)  | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 12       | 1.9           |
| (1,738)  | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 20       | 1.9           |
| (1,642)  | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD11 | 18       | 1.9           |
| (1,638)  | 1:639:A:MET:HA   | 1:652:A:LEU:HD22 | 7        | 1.9           |
| (1,524)  | 1:595:A:VAL:HG23 | 1:646:A:ARG:HD3  | 6        | 1.9           |
| (1,523)  | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD2  | 6        | 1.9           |
| (1,423)  | 1:629:A:VAL:HG13 | 1:626:A:GLU:HG2  | 6        | 1.9           |
| (1,394)  | 1:635:A:VAL:HG13 | 1:632:A:ALA:HA   | 1        | 1.9           |
| (1,394)  | 1:635:A:VAL:HG13 | 1:632:A:ALA:HA   | 3        | 1.9           |
| (1,318)  | 1:652:A:LEU:HA   | 1:652:A:LEU:HD12 | 9        | 1.9           |
| (1,303)  | 1:664:A:LEU:HD12 | 1:664:A:LEU:HA   | 15       | 1.9           |
| (1,248)  | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 14       | 1.9           |
| (1,5)    | 1:608:A:VAL:HG23 | 1:625:A:MET:HE3  | 9        | 1.9           |
| (1,495)  | 1:653:A:LEU:HD11 | 1:603:A:LEU:HD13 | 5        | 1.89          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,462)  | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 14       | 1.89          |
| (1,368)  | 1:653:A:LEU:HA   | 1:653:A:LEU:HD21 | 16       | 1.89          |
| (1,278)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 7        | 1.89          |
| (1,278)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 9        | 1.89          |
| (1,121)  | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE1  | 2        | 1.89          |
| (1,121)  | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE2  | 2        | 1.89          |
| (1,116)  | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD1  | 2        | 1.89          |
| (1,116)  | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD2  | 2        | 1.89          |
| (1,31)   | 1:639:A:MET:HB2  | 1:643:A:ALA:HB2  | 13       | 1.89          |
| (1,559)  | 1:603:A:LEU:HD21 | 1:600:A:ARG:HA   | 9        | 1.88          |
| (1,348)  | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD12 | 3        | 1.88          |
| (1,345)  | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD13 | 3        | 1.88          |
| (1,294)  | 1:604:A:VAL:HG11 | 1:633:A:LYS:HD2  | 1        | 1.88          |
| (1,278)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 3        | 1.88          |
| (1,278)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 4        | 1.88          |
| (1,278)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 6        | 1.88          |
| (1,278)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 19       | 1.88          |
| (1,46)   | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 19       | 1.88          |
| (1,31)   | 1:639:A:MET:HB2  | 1:643:A:ALA:HB2  | 3        | 1.88          |
| (1,6)    | 1:608:A:VAL:HG11 | 1:625:A:MET:HE3  | 20       | 1.88          |
| (2,75)   | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 18       | 1.87          |
| (2,75)   | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 18       | 1.87          |
| (2,75)   | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 18       | 1.87          |
| (2,75)   | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 18       | 1.87          |
| (2,75)   | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 18       | 1.87          |
| (2,75)   | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 18       | 1.87          |
| (1,640)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD11 | 2        | 1.87          |
| (1,638)  | 1:639:A:MET:HA   | 1:652:A:LEU:HD21 | 15       | 1.87          |
| (1,625)  | 1:632:A:ALA:HB2  | 1:628:A:LEU:HD12 | 3        | 1.87          |
| (1,600)  | 1:646:A:ARG:HA   | 1:595:A:VAL:HG22 | 9        | 1.87          |
| (1,499)  | 1:639:A:MET:HG3  | 1:652:A:LEU:HD22 | 18       | 1.87          |
| (1,318)  | 1:652:A:LEU:HA   | 1:652:A:LEU:HD13 | 2        | 1.87          |
| (1,318)  | 1:652:A:LEU:HA   | 1:652:A:LEU:HD11 | 17       | 1.87          |
| (1,303)  | 1:664:A:LEU:HD11 | 1:664:A:LEU:HA   | 2        | 1.87          |
| (1,278)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 13       | 1.87          |
| (1,278)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 15       | 1.87          |
| (1,98)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 14       | 1.87          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 15       | 1.86          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 15       | 1.86          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 15       | 1.86          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 14       | 1.86          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 14       | 1.86          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 14       | 1.86          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 14       | 1.86          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 14       | 1.86          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 14       | 1.86          |
| (1,626)  | 1:625:A:MET:HE1  | 1:628:A:LEU:HD12 | 2        | 1.86          |
| (1,523)  | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD2  | 9        | 1.86          |
| (1,394)  | 1:635:A:VAL:HG13 | 1:632:A:ALA:HA   | 17       | 1.86          |
| (1,368)  | 1:653:A:LEU:HA   | 1:653:A:LEU:HD22 | 4        | 1.86          |
| (1,318)  | 1:652:A:LEU:HA   | 1:652:A:LEU:HD13 | 10       | 1.86          |
| (1,318)  | 1:652:A:LEU:HA   | 1:652:A:LEU:HD13 | 11       | 1.86          |
| (1,318)  | 1:652:A:LEU:HA   | 1:652:A:LEU:HD12 | 14       | 1.86          |
| (1,318)  | 1:652:A:LEU:HA   | 1:652:A:LEU:HD13 | 20       | 1.86          |
| (1,248)  | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 5        | 1.86          |
| (1,24)   | 1:650:A:TYR:HA   | 1:653:A:LEU:HD11 | 2        | 1.86          |
| (1,24)   | 1:650:A:TYR:HA   | 1:653:A:LEU:HD13 | 20       | 1.86          |
| (3,27)   | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD1  | 1        | 1.85          |
| (3,27)   | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD2  | 1        | 1.85          |
| (3,27)   | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD1  | 1        | 1.85          |
| (3,27)   | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD2  | 1        | 1.85          |
| (3,27)   | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD1  | 1        | 1.85          |
| (3,27)   | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD2  | 1        | 1.85          |
| (3,22)   | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE1  | 9        | 1.85          |
| (3,22)   | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE2  | 9        | 1.85          |
| (3,22)   | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE1  | 9        | 1.85          |
| (3,22)   | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE2  | 9        | 1.85          |
| (3,22)   | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE1  | 9        | 1.85          |
| (3,22)   | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE2  | 9        | 1.85          |
| (2,75)   | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 1        | 1.85          |
| (2,75)   | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 1        | 1.85          |
| (2,75)   | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 1        | 1.85          |
| (2,75)   | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 1        | 1.85          |
| (2,75)   | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 1        | 1.85          |
| (2,75)   | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 1        | 1.85          |
| (1,638)  | 1:639:A:MET:HA   | 1:652:A:LEU:HD23 | 2        | 1.85          |
| (1,625)  | 1:632:A:ALA:HB2  | 1:628:A:LEU:HD13 | 7        | 1.85          |
| (1,597)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HD1  | 16       | 1.85          |
| (1,597)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HD2  | 16       | 1.85          |
| (1,394)  | 1:635:A:VAL:HG12 | 1:632:A:ALA:HA   | 2        | 1.85          |
| (1,394)  | 1:635:A:VAL:HG12 | 1:632:A:ALA:HA   | 20       | 1.85          |
| (1,116)  | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD1  | 8        | 1.85          |
| (1,116)  | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD2  | 8        | 1.85          |
| (1,46)   | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 15       | 1.85          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,4)   | 1:629:A:VAL:HG21 | 1:625:A:MET:HE3  | 9        | 1.85          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 7        | 1.84          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 7        | 1.84          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 7        | 1.84          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 11       | 1.84          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 11       | 1.84          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 11       | 1.84          |
| (1,738) | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 11       | 1.84          |
| (1,738) | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 17       | 1.84          |
| (1,559) | 1:603:A:LEU:HD22 | 1:600:A:ARG:HA   | 8        | 1.84          |
| (1,536) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD23 | 5        | 1.84          |
| (1,535) | 1:639:A:MET:HG3  | 1:653:A:LEU:HD21 | 10       | 1.84          |
| (1,467) | 1:652:A:LEU:HD22 | 1:643:A:ALA:HA   | 4        | 1.84          |
| (1,433) | 1:656:A:LYS:HG2  | 1:639:A:MET:HE2  | 10       | 1.84          |
| (1,394) | 1:635:A:VAL:HG11 | 1:632:A:ALA:HA   | 6        | 1.84          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD22 | 4        | 1.84          |
| (1,318) | 1:652:A:LEU:HA   | 1:652:A:LEU:HD12 | 3        | 1.84          |
| (1,294) | 1:604:A:VAL:HG11 | 1:633:A:LYS:HD2  | 20       | 1.84          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 6        | 1.83          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 6        | 1.83          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 6        | 1.83          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 6        | 1.83          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 6        | 1.83          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 6        | 1.83          |
| (1,573) | 1:657:A:ILE:HD11 | 1:606:A:LYS:HG2  | 12       | 1.83          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB2  | 15       | 1.83          |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD21 | 17       | 1.83          |
| (1,303) | 1:664:A:LEU:HD12 | 1:664:A:LEU:HA   | 11       | 1.83          |
| (1,229) | 1:636:A:GLU:HG2  | 1:604:A:VAL:HG22 | 19       | 1.83          |
| (1,927) | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 3        | 1.82          |
| (1,623) | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD12 | 5        | 1.82          |
| (1,617) | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 2        | 1.82          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB1  | 2        | 1.82          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB1  | 8        | 1.82          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB1  | 14       | 1.82          |
| (1,294) | 1:604:A:VAL:HG11 | 1:633:A:LYS:HD2  | 4        | 1.82          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE1  | 3        | 1.82          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE2  | 3        | 1.82          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 4        | 1.82          |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD11 | 7        | 1.82          |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD22 | 9        | 1.81          |
| (1,617) | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 17       | 1.81          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG22 | 8        | 1.81          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD11 | 14       | 1.81          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB2  | 6        | 1.81          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB1  | 20       | 1.81          |
| (1,394) | 1:635:A:VAL:HG12 | 1:632:A:ALA:HA   | 8        | 1.81          |
| (1,278) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 1        | 1.81          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 8        | 1.81          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB1  | 5        | 1.81          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB1  | 12       | 1.81          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 5        | 1.8           |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 5        | 1.8           |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 5        | 1.8           |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 5        | 1.8           |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 5        | 1.8           |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 5        | 1.8           |
| (1,640) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD12 | 17       | 1.8           |
| (1,573) | 1:657:A:ILE:HD12 | 1:606:A:LYS:HG2  | 15       | 1.8           |
| (1,366) | 1:639:A:MET:HE2  | 1:653:A:LEU:HD21 | 19       | 1.8           |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD12 | 7        | 1.8           |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 17       | 1.8           |
| (1,639) | 1:652:A:LEU:HD22 | 1:642:A:SER:HB2  | 10       | 1.79          |
| (1,637) | 1:642:A:SER:HB2  | 1:639:A:MET:HA   | 1        | 1.79          |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG21 | 3        | 1.79          |
| (1,406) | 1:635:A:VAL:HG23 | 1:656:A:LYS:HG2  | 16       | 1.79          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB2  | 11       | 1.79          |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 16       | 1.79          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD12 | 12       | 1.78          |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG23 | 17       | 1.78          |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE2  | 19       | 1.78          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB2  | 4        | 1.78          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB2  | 13       | 1.78          |
| (1,294) | 1:604:A:VAL:HG12 | 1:633:A:LYS:HD2  | 9        | 1.78          |
| (1,208) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD13 | 13       | 1.78          |
| (1,202) | 1:620:A:LEU:HD21 | 1:620:A:LEU:HA   | 15       | 1.78          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE1  | 19       | 1.78          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE2  | 19       | 1.78          |
| (1,87)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 3        | 1.78          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 5        | 1.78          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 11       | 1.78          |
| (1,4)   | 1:629:A:VAL:HG21 | 1:625:A:MET:HE3  | 3        | 1.78          |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD22 | 5        | 1.77          |
| (1,484) | 1:607:A:LEU:HD23 | 1:653:A:LEU:HB2  | 17       | 1.77          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD22 | 13       | 1.77          |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 5        | 1.77          |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 17       | 1.77          |
| (3,21)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD1  | 20       | 1.76          |
| (3,21)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD2  | 20       | 1.76          |
| (3,21)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD1  | 20       | 1.76          |
| (3,21)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD2  | 20       | 1.76          |
| (3,21)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD1  | 20       | 1.76          |
| (3,21)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD2  | 20       | 1.76          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD13 | 15       | 1.76          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB2  | 9        | 1.76          |
| (1,394) | 1:635:A:VAL:HG12 | 1:632:A:ALA:HA   | 4        | 1.76          |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD12 | 1        | 1.76          |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD12 | 9        | 1.76          |
| (1,294) | 1:604:A:VAL:HG13 | 1:633:A:LYS:HD2  | 7        | 1.76          |
| (1,207) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD11 | 14       | 1.76          |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 6        | 1.76          |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 8        | 1.76          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 4        | 1.75          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 4        | 1.75          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 4        | 1.75          |
| (1,637) | 1:642:A:SER:HB2  | 1:639:A:MET:HA   | 20       | 1.75          |
| (1,547) | 1:603:A:LEU:HD12 | 1:606:A:LYS:HD2  | 12       | 1.75          |
| (1,423) | 1:629:A:VAL:HG13 | 1:626:A:GLU:HG2  | 2        | 1.75          |
| (1,423) | 1:629:A:VAL:HG12 | 1:626:A:GLU:HG2  | 9        | 1.75          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB1  | 16       | 1.75          |
| (1,394) | 1:635:A:VAL:HG13 | 1:632:A:ALA:HA   | 7        | 1.75          |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD21 | 7        | 1.75          |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD12 | 16       | 1.75          |
| (1,294) | 1:604:A:VAL:HG12 | 1:633:A:LYS:HD2  | 14       | 1.75          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 1        | 1.75          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 1        | 1.75          |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 15       | 1.75          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 1        | 1.75          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 9        | 1.75          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB3  | 15       | 1.75          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB1  | 3        | 1.74          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB2  | 5        | 1.74          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB3  | 7        | 1.74          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB3  | 17       | 1.74          |
| (1,171) | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 13       | 1.74          |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 4        | 1.74          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE1  | 2        | 1.73          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE2  | 2        | 1.73          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE1  | 2        | 1.73          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE2  | 2        | 1.73          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE1  | 2        | 1.73          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE2  | 2        | 1.73          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 2        | 1.73          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 8        | 1.73          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 8        | 1.73          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 8        | 1.73          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 8        | 1.73          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 8        | 1.73          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 8        | 1.73          |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 19       | 1.73          |
| (1,617) | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 12       | 1.73          |
| (1,603) | 1:599:A:LEU:HD11 | 1:595:A:VAL:HG13 | 4        | 1.73          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 15       | 1.73          |
| (1,536) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD23 | 13       | 1.73          |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 14       | 1.73          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE3  | 5        | 1.73          |
| (1,4)   | 1:629:A:VAL:HG21 | 1:625:A:MET:HE3  | 14       | 1.73          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD1  | 17       | 1.72          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD2  | 17       | 1.72          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD1  | 17       | 1.72          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD2  | 17       | 1.72          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD1  | 17       | 1.72          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD2  | 17       | 1.72          |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 5        | 1.72          |
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD12 | 13       | 1.72          |
| (1,639) | 1:652:A:LEU:HD23 | 1:642:A:SER:HB2  | 14       | 1.72          |
| (1,637) | 1:642:A:SER:HB2  | 1:639:A:MET:HA   | 12       | 1.72          |
| (1,637) | 1:642:A:SER:HB2  | 1:639:A:MET:HA   | 17       | 1.72          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE2  | 2        | 1.72          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE2  | 19       | 1.72          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 6        | 1.72          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 13       | 1.72          |
| (1,87)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 12       | 1.72          |
| (1,74)  | 1:672:A:LEU:HD12 | 1:672:A:LEU:HA   | 18       | 1.72          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 4        | 1.72          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB1  | 6        | 1.72          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB2  | 7        | 1.72          |
| (1,6)   | 1:608:A:VAL:HG13 | 1:625:A:MET:HE2  | 19       | 1.72          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD11 | 14       | 1.71          |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE2  | 2        | 1.71          |
| (1,423) | 1:629:A:VAL:HG11 | 1:626:A:GLU:HG2  | 10       | 1.71          |
| (1,423) | 1:629:A:VAL:HG13 | 1:626:A:GLU:HG2  | 13       | 1.71          |
| (1,366) | 1:639:A:MET:HE3  | 1:653:A:LEU:HD23 | 5        | 1.71          |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD13 | 2        | 1.71          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 9        | 1.71          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 9        | 1.71          |
| (1,87)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 17       | 1.71          |
| (1,4)   | 1:629:A:VAL:HG21 | 1:625:A:MET:HE2  | 10       | 1.71          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE1  | 19       | 1.7           |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE2  | 19       | 1.7           |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE1  | 19       | 1.7           |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE2  | 19       | 1.7           |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE1  | 19       | 1.7           |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE2  | 19       | 1.7           |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD11 | 15       | 1.7           |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 6        | 1.7           |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 16       | 1.7           |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 16       | 1.7           |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 16       | 1.7           |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 16       | 1.7           |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 16       | 1.7           |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 16       | 1.7           |
| (1,738) | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 15       | 1.7           |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD22 | 17       | 1.7           |
| (1,637) | 1:642:A:SER:HB2  | 1:639:A:MET:HA   | 19       | 1.7           |
| (1,559) | 1:603:A:LEU:HD22 | 1:600:A:ARG:HA   | 5        | 1.7           |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB2  | 17       | 1.7           |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD23 | 6        | 1.7           |
| (1,208) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD13 | 4        | 1.7           |
| (1,141) | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE1  | 16       | 1.7           |
| (1,141) | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE2  | 16       | 1.7           |
| (1,74)  | 1:672:A:LEU:HD11 | 1:672:A:LEU:HA   | 4        | 1.7           |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 13       | 1.7           |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB2  | 20       | 1.7           |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD13 | 14       | 1.7           |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD21 | 18       | 1.69          |
| (1,496) | 1:599:A:LEU:HD13 | 1:603:A:LEU:HD23 | 13       | 1.69          |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD23 | 4        | 1.69          |
| (1,359) | 1:603:A:LEU:HD13 | 1:599:A:LEU:HD21 | 1        | 1.69          |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD12 | 18       | 1.69          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD12 | 19       | 1.69          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB1  | 19       | 1.69          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 5        | 1.69          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 5        | 1.69          |
| (1,71)  | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 17       | 1.69          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 19       | 1.69          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB2  | 18       | 1.69          |
| (1,640) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD13 | 3        | 1.68          |
| (1,637) | 1:642:A:SER:HB2  | 1:639:A:MET:HA   | 3        | 1.68          |
| (1,637) | 1:642:A:SER:HB2  | 1:639:A:MET:HA   | 10       | 1.68          |
| (1,637) | 1:642:A:SER:HB2  | 1:639:A:MET:HA   | 11       | 1.68          |
| (1,637) | 1:642:A:SER:HB2  | 1:639:A:MET:HA   | 18       | 1.68          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 4        | 1.68          |
| (1,559) | 1:603:A:LEU:HD23 | 1:600:A:ARG:HA   | 12       | 1.68          |
| (1,499) | 1:639:A:MET:HG3  | 1:652:A:LEU:HD21 | 5        | 1.68          |
| (1,470) | 1:635:A:VAL:HG11 | 1:639:A:MET:HE2  | 5        | 1.68          |
| (1,406) | 1:635:A:VAL:HG23 | 1:656:A:LYS:HG2  | 4        | 1.68          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB2  | 19       | 1.68          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 10       | 1.68          |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD13 | 3        | 1.68          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 7        | 1.67          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 7        | 1.67          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 7        | 1.67          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 7        | 1.67          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 7        | 1.67          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 7        | 1.67          |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD23 | 8        | 1.67          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD11 | 17       | 1.67          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD11 | 17       | 1.67          |
| (1,617) | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 3        | 1.67          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 13       | 1.67          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 13       | 1.67          |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 18       | 1.67          |
| (1,208) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD12 | 5        | 1.67          |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 4        | 1.67          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB1  | 9        | 1.67          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD11 | 17       | 1.66          |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 13       | 1.66          |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 15       | 1.66          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 15       | 1.66          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 15       | 1.66          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 15       | 1.66          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 15       | 1.66          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 15       | 1.66          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 15       | 1.66          |
| (1,524) | 1:595:A:VAL:HG23 | 1:646:A:ARG:HD3  | 5        | 1.66          |
| (1,492) | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 12       | 1.66          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE2  | 20       | 1.66          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB3  | 10       | 1.66          |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD12 | 11       | 1.66          |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD12 | 16       | 1.66          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 6        | 1.66          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 9        | 1.66          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 14       | 1.66          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 14       | 1.66          |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 5        | 1.66          |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 15       | 1.66          |
| (1,74)  | 1:672:A:LEU:HD12 | 1:672:A:LEU:HA   | 16       | 1.66          |
| (3,6)   | 1:612:A:PHE:HE1  | 2:545:B:LEU:HD21 | 20       | 1.65          |
| (3,6)   | 1:612:A:PHE:HE1  | 2:545:B:LEU:HD22 | 20       | 1.65          |
| (3,6)   | 1:612:A:PHE:HE1  | 2:545:B:LEU:HD23 | 20       | 1.65          |
| (3,6)   | 1:612:A:PHE:HE2  | 2:545:B:LEU:HD21 | 20       | 1.65          |
| (3,6)   | 1:612:A:PHE:HE2  | 2:545:B:LEU:HD22 | 20       | 1.65          |
| (3,6)   | 1:612:A:PHE:HE2  | 2:545:B:LEU:HD23 | 20       | 1.65          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 17       | 1.65          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 8        | 1.65          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 1        | 1.65          |
| (1,359) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD23 | 5        | 1.65          |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD13 | 20       | 1.65          |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD13 | 8        | 1.65          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 16       | 1.65          |
| (1,208) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD11 | 6        | 1.65          |
| (1,74)  | 1:672:A:LEU:HD13 | 1:672:A:LEU:HA   | 10       | 1.65          |
| (1,74)  | 1:672:A:LEU:HD13 | 1:672:A:LEU:HA   | 20       | 1.65          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 7        | 1.65          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 12       | 1.65          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB1  | 10       | 1.65          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB1  | 11       | 1.65          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB3  | 14       | 1.65          |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD13 | 8        | 1.65          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD11 | 5        | 1.64          |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD21 | 4        | 1.64          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD12 | 15       | 1.64          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD12 | 15       | 1.64          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD12 | 11       | 1.64          |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD12 | 11       | 1.64          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 16       | 1.64          |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE1  | 4        | 1.64          |
| (1,423) | 1:629:A:VAL:HG12 | 1:626:A:GLU:HG2  | 17       | 1.64          |
| (1,357) | 1:608:A:VAL:HG23 | 1:629:A:VAL:HA   | 1        | 1.64          |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD12 | 1        | 1.64          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 10       | 1.64          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 12       | 1.64          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 19       | 1.64          |
| (1,148) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE1  | 13       | 1.64          |
| (1,148) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HE2  | 13       | 1.64          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 19       | 1.64          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 19       | 1.64          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 12       | 1.64          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 14       | 1.64          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 2        | 1.64          |
| (1,5)   | 1:608:A:VAL:HG21 | 1:625:A:MET:HE3  | 3        | 1.64          |
| (1,5)   | 1:608:A:VAL:HG23 | 1:625:A:MET:HE3  | 15       | 1.64          |
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD13 | 15       | 1.63          |
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD11 | 16       | 1.63          |
| (1,637) | 1:642:A:SER:HB2  | 1:639:A:MET:HA   | 2        | 1.63          |
| (1,637) | 1:642:A:SER:HB2  | 1:639:A:MET:HA   | 9        | 1.63          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 3        | 1.63          |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD22 | 13       | 1.63          |
| (1,480) | 1:653:A:LEU:HD23 | 1:636:A:GLU:HA   | 13       | 1.63          |
| (1,229) | 1:636:A:GLU:HG2  | 1:604:A:VAL:HG21 | 15       | 1.63          |
| (1,130) | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 7        | 1.63          |
| (1,130) | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 16       | 1.63          |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 12       | 1.63          |
| (1,74)  | 1:672:A:LEU:HD13 | 1:672:A:LEU:HA   | 5        | 1.63          |
| (1,74)  | 1:672:A:LEU:HD11 | 1:672:A:LEU:HA   | 8        | 1.63          |
| (1,74)  | 1:672:A:LEU:HD11 | 1:672:A:LEU:HA   | 11       | 1.63          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB2  | 4        | 1.63          |
| (1,4)   | 1:629:A:VAL:HG23 | 1:625:A:MET:HE1  | 6        | 1.63          |
| (1,738) | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 13       | 1.62          |
| (1,637) | 1:642:A:SER:HB2  | 1:639:A:MET:HA   | 6        | 1.62          |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG21 | 1        | 1.62          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 4        | 1.62          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 17       | 1.62          |
| (1,434) | 1:635:A:VAL:HG23 | 1:639:A:MET:HE2  | 9        | 1.62          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE2  | 9        | 1.62          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD22 | 2        | 1.62          |
| (1,294) | 1:604:A:VAL:HG12 | 1:633:A:LYS:HD2  | 5        | 1.62          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 3        | 1.62          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 5        | 1.62          |
| (1,74)  | 1:672:A:LEU:HD12 | 1:672:A:LEU:HA   | 13       | 1.62          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 17       | 1.62          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 18       | 1.62          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE1  | 20       | 1.61          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE2  | 20       | 1.61          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE1  | 20       | 1.61          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE2  | 20       | 1.61          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE1  | 20       | 1.61          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE2  | 20       | 1.61          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD11 | 20       | 1.61          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 20       | 1.61          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 19       | 1.61          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 19       | 1.61          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 19       | 1.61          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 19       | 1.61          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 19       | 1.61          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 19       | 1.61          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 20       | 1.61          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 20       | 1.61          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 20       | 1.61          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 20       | 1.61          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 20       | 1.61          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 20       | 1.61          |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD22 | 1        | 1.61          |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD23 | 16       | 1.61          |
| (1,610) | 1:599:A:LEU:HD23 | 1:603:A:LEU:HD21 | 11       | 1.61          |
| (1,536) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD22 | 12       | 1.61          |
| (1,536) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD22 | 17       | 1.61          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE2  | 16       | 1.61          |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD21 | 12       | 1.61          |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD23 | 2        | 1.61          |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD22 | 7        | 1.61          |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD23 | 20       | 1.61          |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD11 | 17       | 1.61          |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 7        | 1.61          |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD1  | 4        | 1.61          |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD2  | 4        | 1.61          |
| (1,74)  | 1:672:A:LEU:HD13 | 1:672:A:LEU:HA   | 17       | 1.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,71)   | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 6        | 1.61          |
| (1,70)   | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 4        | 1.61          |
| (1,46)   | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 3        | 1.61          |
| (1,6)    | 1:608:A:VAL:HG13 | 1:625:A:MET:HE1  | 5        | 1.61          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 16       | 1.6           |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 16       | 1.6           |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 16       | 1.6           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 16       | 1.6           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 16       | 1.6           |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 16       | 1.6           |
| (1,626)  | 1:625:A:MET:HE3  | 1:628:A:LEU:HD12 | 20       | 1.6           |
| (1,600)  | 1:646:A:ARG:HA   | 1:595:A:VAL:HG21 | 10       | 1.6           |
| (1,462)  | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 11       | 1.6           |
| (1,394)  | 1:635:A:VAL:HG12 | 1:632:A:ALA:HA   | 14       | 1.6           |
| (1,368)  | 1:653:A:LEU:HA   | 1:653:A:LEU:HD21 | 20       | 1.6           |
| (1,345)  | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD11 | 10       | 1.6           |
| (1,326)  | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 7        | 1.6           |
| (1,315)  | 1:603:A:LEU:HA   | 1:603:A:LEU:HD13 | 14       | 1.6           |
| (1,294)  | 1:604:A:VAL:HG12 | 1:633:A:LYS:HD2  | 11       | 1.6           |
| (1,293)  | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 10       | 1.6           |
| (1,248)  | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 10       | 1.6           |
| (1,229)  | 1:636:A:GLU:HG2  | 1:604:A:VAL:HG21 | 18       | 1.6           |
| (1,208)  | 1:607:A:LEU:HA   | 1:607:A:LEU:HD13 | 19       | 1.6           |
| (1,207)  | 1:632:A:ALA:HA   | 1:607:A:LEU:HD12 | 3        | 1.6           |
| (1,98)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 9        | 1.6           |
| (1,74)   | 1:672:A:LEU:HD13 | 1:672:A:LEU:HA   | 1        | 1.6           |
| (1,74)   | 1:672:A:LEU:HD11 | 1:672:A:LEU:HA   | 7        | 1.6           |
| (1,31)   | 1:639:A:MET:HB2  | 1:643:A:ALA:HB2  | 8        | 1.6           |
| (1,5)    | 1:608:A:VAL:HG21 | 1:625:A:MET:HE2  | 16       | 1.6           |
| (2,111)  | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD11 | 16       | 1.59          |
| (2,111)  | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD12 | 16       | 1.59          |
| (2,111)  | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD13 | 16       | 1.59          |
| (2,111)  | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD11 | 16       | 1.59          |
| (2,111)  | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD12 | 16       | 1.59          |
| (2,111)  | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD13 | 16       | 1.59          |
| (1,738)  | 1:597:A:GLN:HE21 | 1:596:A:THR:HB   | 18       | 1.59          |
| (1,638)  | 1:639:A:MET:HA   | 1:652:A:LEU:HD22 | 11       | 1.59          |
| (1,593)  | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 6        | 1.59          |
| (1,397)  | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB1  | 12       | 1.59          |
| (1,315)  | 1:603:A:LEU:HA   | 1:603:A:LEU:HD11 | 7        | 1.59          |
| (1,315)  | 1:603:A:LEU:HA   | 1:603:A:LEU:HD11 | 18       | 1.59          |
| (1,315)  | 1:603:A:LEU:HA   | 1:603:A:LEU:HD13 | 20       | 1.59          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 9        | 1.59          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 16       | 1.59          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 19       | 1.59          |
| (1,208) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD11 | 10       | 1.59          |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 16       | 1.59          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 11       | 1.58          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 11       | 1.58          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 11       | 1.58          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 11       | 1.58          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 11       | 1.58          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 11       | 1.58          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 14       | 1.58          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 14       | 1.58          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 14       | 1.58          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 14       | 1.58          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 14       | 1.58          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 14       | 1.58          |
| (1,623) | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD11 | 10       | 1.58          |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 15       | 1.58          |
| (1,423) | 1:629:A:VAL:HG11 | 1:626:A:GLU:HG2  | 16       | 1.58          |
| (1,406) | 1:635:A:VAL:HG23 | 1:656:A:LYS:HG2  | 20       | 1.58          |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD22 | 8        | 1.58          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD13 | 5        | 1.58          |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD1  | 19       | 1.58          |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD2  | 19       | 1.58          |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 6        | 1.58          |
| (1,74)  | 1:672:A:LEU:HD13 | 1:672:A:LEU:HA   | 3        | 1.58          |
| (1,4)   | 1:629:A:VAL:HG22 | 1:625:A:MET:HE3  | 4        | 1.58          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD13 | 6        | 1.57          |
| (1,623) | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD11 | 2        | 1.57          |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG21 | 16       | 1.57          |
| (1,536) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD23 | 14       | 1.57          |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 12       | 1.57          |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE1  | 12       | 1.57          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD11 | 1        | 1.57          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD13 | 9        | 1.57          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD13 | 10       | 1.57          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD12 | 15       | 1.57          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 18       | 1.57          |
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD1  | 20       | 1.57          |
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD2  | 20       | 1.57          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 10       | 1.57          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD12 | 18       | 1.56          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 10       | 1.56          |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD11 | 15       | 1.56          |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD11 | 15       | 1.56          |
| (1,470) | 1:635:A:VAL:HG12 | 1:639:A:MET:HE3  | 3        | 1.56          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB3  | 6        | 1.56          |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD22 | 3        | 1.56          |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD12 | 14       | 1.56          |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 5        | 1.56          |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 7        | 1.56          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 7        | 1.56          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 11       | 1.56          |
| (1,208) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD13 | 18       | 1.56          |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 13       | 1.56          |
| (1,74)  | 1:672:A:LEU:HD11 | 1:672:A:LEU:HA   | 15       | 1.56          |
| (1,74)  | 1:672:A:LEU:HD13 | 1:672:A:LEU:HA   | 19       | 1.56          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 6        | 1.56          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD12 | 2        | 1.55          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD11 | 9        | 1.55          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 6        | 1.55          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD11 | 9        | 1.55          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD11 | 9        | 1.55          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 14       | 1.55          |
| (1,547) | 1:603:A:LEU:HD11 | 1:606:A:LYS:HD2  | 19       | 1.55          |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 4        | 1.55          |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 12       | 1.55          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 9        | 1.55          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 13       | 1.55          |
| (1,207) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD11 | 7        | 1.55          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 14       | 1.55          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 15       | 1.55          |
| (1,71)  | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 19       | 1.55          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 20       | 1.55          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB3  | 16       | 1.55          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD13 | 8        | 1.54          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 6        | 1.54          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 14       | 1.54          |
| (1,480) | 1:653:A:LEU:HD21 | 1:636:A:GLU:HA   | 16       | 1.54          |
| (1,423) | 1:629:A:VAL:HG11 | 1:626:A:GLU:HG2  | 7        | 1.54          |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD21 | 3        | 1.54          |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD13 | 20       | 1.54          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD12 | 13       | 1.54          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 8        | 1.54          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 15       | 1.54          |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD1  | 11       | 1.54          |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD2  | 11       | 1.54          |
| (1,71)  | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 13       | 1.54          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB1  | 19       | 1.54          |
| (1,4)   | 1:629:A:VAL:HG21 | 1:625:A:MET:HE2  | 2        | 1.54          |
| (1,640) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD13 | 12       | 1.53          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD11 | 20       | 1.53          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD11 | 20       | 1.53          |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE2  | 20       | 1.53          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE3  | 1        | 1.53          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD11 | 6        | 1.53          |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 13       | 1.53          |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 14       | 1.53          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD1  | 10       | 1.53          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD2  | 10       | 1.53          |
| (1,74)  | 1:672:A:LEU:HD12 | 1:672:A:LEU:HA   | 2        | 1.53          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 20       | 1.52          |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD22 | 18       | 1.52          |
| (1,434) | 1:635:A:VAL:HG21 | 1:639:A:MET:HE1  | 13       | 1.52          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE3  | 7        | 1.52          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB3  | 19       | 1.52          |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD23 | 11       | 1.52          |
| (1,366) | 1:639:A:MET:HE1  | 1:653:A:LEU:HD21 | 6        | 1.52          |
| (1,294) | 1:604:A:VAL:HG13 | 1:633:A:LYS:HD2  | 16       | 1.52          |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 2        | 1.52          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 3        | 1.52          |
| (1,208) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD12 | 1        | 1.52          |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 4        | 1.52          |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 5        | 1.52          |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 18       | 1.52          |
| (1,121) | 1:653:A:LEU:HD12 | 1:649:A:TYR:HE1  | 17       | 1.52          |
| (1,121) | 1:653:A:LEU:HD12 | 1:649:A:TYR:HE2  | 17       | 1.52          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD12 | 11       | 1.51          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 4        | 1.51          |
| (1,812) | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 8        | 1.51          |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG23 | 4        | 1.51          |
| (1,523) | 1:595:A:VAL:HG23 | 1:646:A:ARG:HD2  | 5        | 1.51          |
| (1,496) | 1:599:A:LEU:HD11 | 1:603:A:LEU:HD21 | 9        | 1.51          |
| (1,484) | 1:607:A:LEU:HD21 | 1:653:A:LEU:HB2  | 9        | 1.51          |
| (1,470) | 1:635:A:VAL:HG11 | 1:639:A:MET:HE3  | 14       | 1.51          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 18       | 1.51          |
| (1,406) | 1:635:A:VAL:HG23 | 1:656:A:LYS:HG2  | 8        | 1.51          |
| (1,406) | 1:635:A:VAL:HG21 | 1:656:A:LYS:HG2  | 17       | 1.51          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB1  | 15       | 1.51          |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD23 | 15       | 1.51          |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD13 | 17       | 1.51          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD13 | 16       | 1.51          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 18       | 1.51          |
| (1,207) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD13 | 12       | 1.51          |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 13       | 1.51          |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 14       | 1.51          |
| (1,74)  | 1:672:A:LEU:HD12 | 1:672:A:LEU:HA   | 6        | 1.51          |
| (1,71)  | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 2        | 1.51          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 8        | 1.51          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD11 | 4        | 1.5           |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD13 | 13       | 1.5           |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 3        | 1.5           |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 6        | 1.5           |
| (1,927) | 1:661:A:GLN:HE21 | 1:660:A:ILE:H    | 11       | 1.5           |
| (1,812) | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 12       | 1.5           |
| (1,812) | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 14       | 1.5           |
| (1,610) | 1:599:A:LEU:HD23 | 1:603:A:LEU:HD22 | 5        | 1.5           |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 4        | 1.5           |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 9        | 1.5           |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 19       | 1.5           |
| (1,457) | 1:608:A:VAL:HG22 | 1:605:A:HIS:HA   | 1        | 1.5           |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE3  | 7        | 1.5           |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 3        | 1.5           |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 15       | 1.5           |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 20       | 1.5           |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 1        | 1.5           |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 6        | 1.5           |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 16       | 1.5           |
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD1  | 3        | 1.5           |
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD2  | 3        | 1.5           |
| (1,106) | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 13       | 1.5           |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 7        | 1.49          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 7        | 1.49          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 7        | 1.49          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 7        | 1.49          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 7        | 1.49          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 7        | 1.49          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 7        | 1.49          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 7        | 1.49          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 7        | 1.49          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD13 | 10       | 1.49          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD13 | 16       | 1.49          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 15       | 1.49          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 13       | 1.49          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD1  | 9        | 1.49          |
| (2,75)  | 2:545:B:LEU:HD21 | 2:542:B:PHE:HD2  | 9        | 1.49          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD1  | 9        | 1.49          |
| (2,75)  | 2:545:B:LEU:HD22 | 2:542:B:PHE:HD2  | 9        | 1.49          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD1  | 9        | 1.49          |
| (2,75)  | 2:545:B:LEU:HD23 | 2:542:B:PHE:HD2  | 9        | 1.49          |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG21 | 7        | 1.49          |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD21 | 12       | 1.49          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 9        | 1.49          |
| (1,456) | 1:608:A:VAL:HB   | 1:605:A:HIS:HA   | 17       | 1.49          |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE1  | 17       | 1.49          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD12 | 19       | 1.49          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB1  | 13       | 1.49          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD22 | 13       | 1.49          |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD22 | 12       | 1.49          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD13 | 4        | 1.49          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD13 | 8        | 1.49          |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 16       | 1.49          |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 3        | 1.49          |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 7        | 1.49          |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 9        | 1.49          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 6        | 1.49          |
| (1,5)   | 1:608:A:VAL:HG21 | 1:625:A:MET:HE2  | 2        | 1.49          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD11 | 1        | 1.48          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD13 | 14       | 1.48          |
| (1,659) | 1:652:A:LEU:HB3  | 1:639:A:MET:HE2  | 14       | 1.48          |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD22 | 3        | 1.48          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE1  | 17       | 1.48          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD12 | 9        | 1.48          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD12 | 17       | 1.48          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD13 | 17       | 1.48          |
| (1,294) | 1:604:A:VAL:HG12 | 1:633:A:LYS:HD2  | 19       | 1.48          |
| (1,278) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 10       | 1.48          |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 12       | 1.48          |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 19       | 1.48          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD1  | 13       | 1.48          |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD2  | 13       | 1.48          |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 17       | 1.48          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 16       | 1.48          |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 8        | 1.48          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD11 | 19       | 1.47          |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD22 | 19       | 1.47          |
| (1,951) | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 9        | 1.47          |
| (1,724) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HD2  | 6        | 1.47          |
| (1,621) | 1:628:A:LEU:HD11 | 1:628:A:LEU:HA   | 13       | 1.47          |
| (1,621) | 1:628:A:LEU:HD12 | 1:628:A:LEU:HA   | 18       | 1.47          |
| (1,496) | 1:599:A:LEU:HD11 | 1:603:A:LEU:HD22 | 10       | 1.47          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 20       | 1.47          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 15       | 1.47          |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 5        | 1.47          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB1  | 11       | 1.47          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB3  | 18       | 1.47          |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD11 | 10       | 1.47          |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 1        | 1.47          |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 17       | 1.47          |
| (1,263) | 1:607:A:LEU:HD22 | 1:632:A:ALA:HB2  | 13       | 1.47          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 10       | 1.47          |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 2        | 1.47          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 3        | 1.47          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 11       | 1.46          |
| (1,621) | 1:628:A:LEU:HD12 | 1:628:A:LEU:HA   | 14       | 1.46          |
| (1,496) | 1:599:A:LEU:HD11 | 1:603:A:LEU:HD22 | 5        | 1.46          |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE2  | 16       | 1.46          |
| (1,366) | 1:639:A:MET:HE2  | 1:653:A:LEU:HD21 | 9        | 1.46          |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD23 | 8        | 1.46          |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD12 | 11       | 1.46          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD11 | 3        | 1.46          |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 6        | 1.46          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 2        | 1.46          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 9        | 1.46          |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 8        | 1.46          |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 17       | 1.46          |
| (3,21)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD1  | 14       | 1.45          |
| (3,21)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD2  | 14       | 1.45          |
| (3,21)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD1  | 14       | 1.45          |
| (3,21)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD2  | 14       | 1.45          |
| (3,21)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD1  | 14       | 1.45          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,21)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD2  | 14       | 1.45          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 13       | 1.45          |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 2        | 1.45          |
| (1,621) | 1:628:A:LEU:HD12 | 1:628:A:LEU:HA   | 8        | 1.45          |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 8        | 1.45          |
| (1,423) | 1:629:A:VAL:HG11 | 1:626:A:GLU:HG2  | 4        | 1.45          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB3  | 2        | 1.45          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB1  | 8        | 1.45          |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD22 | 11       | 1.45          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 1        | 1.45          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 16       | 1.45          |
| (1,106) | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 5        | 1.45          |
| (1,106) | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 6        | 1.45          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE1  | 18       | 1.44          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE2  | 18       | 1.44          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE1  | 18       | 1.44          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE2  | 18       | 1.44          |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE1  | 18       | 1.44          |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE2  | 18       | 1.44          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD11 | 7        | 1.44          |
| (2,1)   | 2:542:B:PHE:HA   | 2:545:B:LEU:HD11 | 7        | 1.44          |
| (2,1)   | 2:542:B:PHE:HA   | 2:545:B:LEU:HD12 | 7        | 1.44          |
| (2,1)   | 2:542:B:PHE:HA   | 2:545:B:LEU:HD13 | 7        | 1.44          |
| (1,628) | 1:608:A:VAL:HA   | 1:628:A:LEU:HD22 | 7        | 1.44          |
| (1,621) | 1:628:A:LEU:HD11 | 1:628:A:LEU:HA   | 2        | 1.44          |
| (1,621) | 1:628:A:LEU:HD11 | 1:628:A:LEU:HA   | 9        | 1.44          |
| (1,610) | 1:599:A:LEU:HD22 | 1:603:A:LEU:HD22 | 19       | 1.44          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 9        | 1.44          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 19       | 1.44          |
| (1,470) | 1:635:A:VAL:HG11 | 1:639:A:MET:HE3  | 4        | 1.44          |
| (1,423) | 1:629:A:VAL:HG12 | 1:626:A:GLU:HG2  | 12       | 1.44          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB1  | 16       | 1.44          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB1  | 17       | 1.44          |
| (1,360) | 1:599:A:LEU:HA   | 1:599:A:LEU:HD21 | 19       | 1.44          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD11 | 11       | 1.44          |
| (1,293) | 1:633:A:LYS:HA   | 1:633:A:LYS:HD2  | 11       | 1.44          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 2        | 1.44          |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD13 | 4        | 1.44          |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 4        | 1.43          |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 11       | 1.43          |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 14       | 1.43          |
| (1,406) | 1:635:A:VAL:HG23 | 1:656:A:LYS:HG2  | 1        | 1.43          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 8        | 1.43          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 5        | 1.43          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 6        | 1.43          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 12       | 1.43          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 20       | 1.43          |
| (1,106) | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 1        | 1.43          |
| (1,106) | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 15       | 1.43          |
| (1,6)   | 1:608:A:VAL:HG11 | 1:625:A:MET:HE3  | 12       | 1.43          |
| (3,7)   | 1:612:A:PHE:HE1  | 2:546:B:LEU:HD21 | 3        | 1.42          |
| (3,7)   | 1:612:A:PHE:HE1  | 2:546:B:LEU:HD22 | 3        | 1.42          |
| (3,7)   | 1:612:A:PHE:HE1  | 2:546:B:LEU:HD23 | 3        | 1.42          |
| (3,7)   | 1:612:A:PHE:HE2  | 2:546:B:LEU:HD21 | 3        | 1.42          |
| (3,7)   | 1:612:A:PHE:HE2  | 2:546:B:LEU:HD22 | 3        | 1.42          |
| (3,7)   | 1:612:A:PHE:HE2  | 2:546:B:LEU:HD23 | 3        | 1.42          |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD23 | 18       | 1.42          |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 2        | 1.42          |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 6        | 1.42          |
| (1,621) | 1:628:A:LEU:HD13 | 1:628:A:LEU:HA   | 4        | 1.42          |
| (1,621) | 1:628:A:LEU:HD13 | 1:628:A:LEU:HA   | 16       | 1.42          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 18       | 1.42          |
| (1,573) | 1:657:A:ILE:HD12 | 1:606:A:LYS:HG2  | 4        | 1.42          |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 16       | 1.42          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD11 | 20       | 1.42          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB1  | 7        | 1.42          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD11 | 19       | 1.42          |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 2        | 1.42          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 17       | 1.42          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 18       | 1.42          |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD21 | 5        | 1.41          |
| (1,434) | 1:635:A:VAL:HG21 | 1:639:A:MET:HE2  | 18       | 1.41          |
| (1,406) | 1:635:A:VAL:HG23 | 1:656:A:LYS:HG2  | 2        | 1.41          |
| (1,302) | 1:614:A:THR:HG21 | 1:617:A:PRO:HA   | 12       | 1.41          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 4        | 1.41          |
| (1,106) | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 17       | 1.41          |
| (1,106) | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 20       | 1.41          |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 2        | 1.41          |
| (1,71)  | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 15       | 1.41          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 5        | 1.41          |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD22 | 7        | 1.4           |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 8        | 1.4           |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 15       | 1.4           |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 11       | 1.4           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 18       | 1.4           |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD12 | 8        | 1.4           |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD12 | 8        | 1.4           |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 10       | 1.4           |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 3        | 1.4           |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 7        | 1.4           |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 8        | 1.4           |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 14       | 1.4           |
| (1,46)  | 1:600:A:ARG:HG2  | 1:597:A:GLN:HA   | 16       | 1.4           |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB3  | 1        | 1.4           |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 20       | 1.39          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 20       | 1.39          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 20       | 1.39          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 20       | 1.39          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 20       | 1.39          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 20       | 1.39          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 20       | 1.39          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 20       | 1.39          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 20       | 1.39          |
| (3,7)   | 1:612:A:PHE:HE1  | 2:546:B:LEU:HD21 | 6        | 1.39          |
| (3,7)   | 1:612:A:PHE:HE1  | 2:546:B:LEU:HD22 | 6        | 1.39          |
| (3,7)   | 1:612:A:PHE:HE1  | 2:546:B:LEU:HD23 | 6        | 1.39          |
| (3,7)   | 1:612:A:PHE:HE2  | 2:546:B:LEU:HD21 | 6        | 1.39          |
| (3,7)   | 1:612:A:PHE:HE2  | 2:546:B:LEU:HD22 | 6        | 1.39          |
| (3,7)   | 1:612:A:PHE:HE2  | 2:546:B:LEU:HD23 | 6        | 1.39          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 7        | 1.39          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD1  | 11       | 1.39          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD2  | 11       | 1.39          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD1  | 11       | 1.39          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD2  | 11       | 1.39          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD1  | 11       | 1.39          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD2  | 11       | 1.39          |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD22 | 3        | 1.39          |
| (1,857) | 1:636:A:GLU:H    | 1:635:A:VAL:HG23 | 13       | 1.39          |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 1        | 1.39          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD11 | 14       | 1.39          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD11 | 14       | 1.39          |
| (1,621) | 1:628:A:LEU:HD12 | 1:628:A:LEU:HA   | 1        | 1.39          |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD11 | 13       | 1.39          |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD11 | 13       | 1.39          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 5        | 1.39          |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE1  | 1        | 1.39          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,435) | 1:653:A:LEU:HD13 | 1:639:A:MET:HE1  | 14       | 1.39          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB1  | 1        | 1.39          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB2  | 5        | 1.39          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB3  | 9        | 1.39          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 8        | 1.39          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 11       | 1.39          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 15       | 1.39          |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE1  | 16       | 1.39          |
| (1,142) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HE2  | 16       | 1.39          |
| (1,31)  | 1:639:A:MET:HB2  | 1:643:A:ALA:HB1  | 17       | 1.39          |
| (1,5)   | 1:608:A:VAL:HG23 | 1:625:A:MET:HE3  | 14       | 1.39          |
| (1,1)   | 1:656:A:LYS:HE2  | 1:639:A:MET:HE1  | 9        | 1.39          |
| (1,992) | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 13       | 1.38          |
| (1,991) | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 13       | 1.38          |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD23 | 12       | 1.38          |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 9        | 1.38          |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 5        | 1.38          |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD11 | 13       | 1.38          |
| (1,141) | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE1  | 3        | 1.38          |
| (1,141) | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE2  | 3        | 1.38          |
| (1,130) | 1:648:A:GLU:HG2  | 1:649:A:TYR:HA   | 10       | 1.38          |
| (1,106) | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 19       | 1.38          |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 10       | 1.38          |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 19       | 1.38          |
| (1,87)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 8        | 1.38          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 7        | 1.38          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD1  | 10       | 1.37          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD2  | 10       | 1.37          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD1  | 10       | 1.37          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD2  | 10       | 1.37          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD1  | 10       | 1.37          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD2  | 10       | 1.37          |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 7        | 1.37          |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 20       | 1.37          |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 4        | 1.37          |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 6        | 1.37          |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 12       | 1.37          |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD12 | 6        | 1.37          |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD12 | 6        | 1.37          |
| (1,581) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 17       | 1.37          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE1  | 4        | 1.37          |
| (1,406) | 1:635:A:VAL:HG21 | 1:656:A:LYS:HG2  | 3        | 1.37          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB2  | 1        | 1.37          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 14       | 1.37          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 14       | 1.37          |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 18       | 1.37          |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 3        | 1.37          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 1        | 1.37          |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD13 | 5        | 1.37          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE1  | 10       | 1.36          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE2  | 10       | 1.36          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE1  | 10       | 1.36          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE2  | 10       | 1.36          |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE1  | 10       | 1.36          |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE2  | 10       | 1.36          |
| (2,105) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB3  | 2        | 1.36          |
| (1,929) | 1:661:A:GLN:HE22 | 1:611:A:ILE:HA   | 12       | 1.36          |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 3        | 1.36          |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 1        | 1.36          |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 4        | 1.36          |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 19       | 1.36          |
| (1,639) | 1:652:A:LEU:HD21 | 1:642:A:SER:HB2  | 20       | 1.36          |
| (1,621) | 1:628:A:LEU:HD12 | 1:628:A:LEU:HA   | 5        | 1.36          |
| (1,621) | 1:628:A:LEU:HD11 | 1:628:A:LEU:HA   | 10       | 1.36          |
| (1,470) | 1:635:A:VAL:HG13 | 1:639:A:MET:HE1  | 16       | 1.36          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 17       | 1.36          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 12       | 1.36          |
| (1,294) | 1:604:A:VAL:HG12 | 1:633:A:LYS:HD2  | 12       | 1.36          |
| (1,183) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HA   | 15       | 1.36          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD11 | 1        | 1.36          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD11 | 1        | 1.36          |
| (1,106) | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 18       | 1.36          |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD21 | 14       | 1.35          |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 12       | 1.35          |
| (1,724) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HD2  | 5        | 1.35          |
| (1,638) | 1:639:A:MET:HA   | 1:652:A:LEU:HD23 | 19       | 1.35          |
| (1,581) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 18       | 1.35          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 12       | 1.35          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD13 | 4        | 1.35          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD12 | 8        | 1.35          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD21 | 9        | 1.35          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 3        | 1.35          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 11       | 1.35          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 16       | 1.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,106)  | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 11       | 1.35          |
| (1,70)   | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 15       | 1.35          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 17       | 1.34          |
| (1,817)  | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 1        | 1.34          |
| (1,817)  | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 17       | 1.34          |
| (1,817)  | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 19       | 1.34          |
| (1,793)  | 1:618:A:ALA:H    | 1:617:A:PRO:HG2  | 2        | 1.34          |
| (1,636)  | 1:639:A:MET:HE2  | 1:639:A:MET:HA   | 5        | 1.34          |
| (1,581)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 9        | 1.34          |
| (1,470)  | 1:635:A:VAL:HG12 | 1:639:A:MET:HE3  | 1        | 1.34          |
| (1,461)  | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 1        | 1.34          |
| (1,417)  | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD13 | 7        | 1.34          |
| (1,406)  | 1:635:A:VAL:HG23 | 1:656:A:LYS:HG2  | 7        | 1.34          |
| (1,348)  | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD12 | 14       | 1.34          |
| (1,263)  | 1:607:A:LEU:HD22 | 1:632:A:ALA:HB1  | 4        | 1.34          |
| (1,106)  | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 3        | 1.34          |
| (1,87)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 13       | 1.34          |
| (1,13)   | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 2        | 1.34          |
| (1,983)  | 1:607:A:LEU:H    | 1:607:A:LEU:HD23 | 1        | 1.33          |
| (1,715)  | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 18       | 1.33          |
| (1,686)  | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 15       | 1.33          |
| (1,686)  | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 17       | 1.33          |
| (1,624)  | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD13 | 19       | 1.33          |
| (1,624)  | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD13 | 19       | 1.33          |
| (1,581)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 11       | 1.33          |
| (1,573)  | 1:657:A:ILE:HD13 | 1:606:A:LYS:HG2  | 19       | 1.33          |
| (1,417)  | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD11 | 1        | 1.33          |
| (1,406)  | 1:635:A:VAL:HG21 | 1:656:A:LYS:HG2  | 14       | 1.33          |
| (1,368)  | 1:653:A:LEU:HA   | 1:653:A:LEU:HD23 | 19       | 1.33          |
| (1,315)  | 1:603:A:LEU:HA   | 1:603:A:LEU:HD12 | 2        | 1.33          |
| (1,148)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HE1  | 12       | 1.33          |
| (1,148)  | 1:635:A:VAL:HG11 | 1:631:A:TYR:HE2  | 12       | 1.33          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 19       | 1.32          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 19       | 1.32          |
| (1,1001) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 19       | 1.32          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD21 | 19       | 1.32          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD22 | 19       | 1.32          |
| (1,1000) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD23 | 19       | 1.32          |
| (1,983)  | 1:607:A:LEU:H    | 1:607:A:LEU:HD23 | 10       | 1.32          |
| (1,817)  | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 5        | 1.32          |
| (1,817)  | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 10       | 1.32          |
| (1,817)  | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 13       | 1.32          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,793) | 1:618:A:ALA:H    | 1:617:A:PRO:HG2  | 12       | 1.32          |
| (1,793) | 1:618:A:ALA:H    | 1:617:A:PRO:HG2  | 16       | 1.32          |
| (1,719) | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 11       | 1.32          |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 10       | 1.32          |
| (1,484) | 1:607:A:LEU:HD23 | 1:653:A:LEU:HB2  | 12       | 1.32          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 11       | 1.32          |
| (1,470) | 1:635:A:VAL:HG11 | 1:639:A:MET:HE1  | 20       | 1.32          |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB3  | 4        | 1.32          |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD12 | 13       | 1.32          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 1        | 1.32          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 5        | 1.32          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 13       | 1.32          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB2  | 8        | 1.32          |
| (1,87)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 4        | 1.32          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 6        | 1.32          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 13       | 1.31          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 13       | 1.31          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 13       | 1.31          |
| (1,742) | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 12       | 1.31          |
| (1,719) | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 10       | 1.31          |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 8        | 1.31          |
| (1,621) | 1:628:A:LEU:HD12 | 1:628:A:LEU:HA   | 17       | 1.31          |
| (1,621) | 1:628:A:LEU:HD11 | 1:628:A:LEU:HA   | 19       | 1.31          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 6        | 1.31          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 7        | 1.31          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 17       | 1.31          |
| (1,456) | 1:608:A:VAL:HB   | 1:605:A:HIS:HA   | 7        | 1.31          |
| (1,366) | 1:639:A:MET:HE1  | 1:653:A:LEU:HD23 | 3        | 1.31          |
| (1,366) | 1:639:A:MET:HE3  | 1:653:A:LEU:HD22 | 13       | 1.31          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 1        | 1.31          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 10       | 1.31          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 13       | 1.31          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 2        | 1.31          |
| (1,32)  | 1:648:A:GLU:HB2  | 1:643:A:ALA:HB3  | 10       | 1.31          |
| (1,4)   | 1:629:A:VAL:HG22 | 1:625:A:MET:HE2  | 16       | 1.31          |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 18       | 1.3           |
| (1,793) | 1:618:A:ALA:H    | 1:617:A:PRO:HG2  | 9        | 1.3           |
| (1,793) | 1:618:A:ALA:H    | 1:617:A:PRO:HG2  | 17       | 1.3           |
| (1,742) | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 8        | 1.3           |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 9        | 1.3           |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 16       | 1.3           |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 2        | 1.3           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 17       | 1.3           |
| (1,248) | 1:659:A:LYS:HA   | 1:659:A:LYS:HE2  | 4        | 1.3           |
| (1,817) | 1:626:A:GLU:H    | 1:625:A:MET:HB2  | 16       | 1.29          |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 6        | 1.29          |
| (1,639) | 1:652:A:LEU:HD22 | 1:642:A:SER:HB2  | 15       | 1.29          |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE1  | 14       | 1.29          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 8        | 1.29          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 15       | 1.29          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 20       | 1.29          |
| (1,286) | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 2        | 1.29          |
| (1,106) | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 14       | 1.29          |
| (1,5)   | 1:608:A:VAL:HG23 | 1:625:A:MET:HE1  | 6        | 1.29          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD11 | 12       | 1.28          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD12 | 12       | 1.28          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD13 | 12       | 1.28          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD11 | 12       | 1.28          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD12 | 12       | 1.28          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD13 | 12       | 1.28          |
| (1,742) | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 2        | 1.28          |
| (1,742) | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 11       | 1.28          |
| (1,742) | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 20       | 1.28          |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 3        | 1.28          |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 16       | 1.28          |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 20       | 1.28          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD11 | 2        | 1.28          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD11 | 2        | 1.28          |
| (1,610) | 1:599:A:LEU:HD23 | 1:603:A:LEU:HD23 | 17       | 1.28          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 18       | 1.28          |
| (1,484) | 1:607:A:LEU:HD22 | 1:653:A:LEU:HB2  | 3        | 1.28          |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE1  | 11       | 1.28          |
| (1,229) | 1:636:A:GLU:HG2  | 1:604:A:VAL:HG21 | 10       | 1.28          |
| (1,190) | 1:601:A:SER:HB2  | 1:598:A:ASP:HA   | 19       | 1.28          |
| (1,141) | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE1  | 12       | 1.28          |
| (1,141) | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE2  | 12       | 1.28          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 15       | 1.27          |
| (1,742) | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 3        | 1.27          |
| (1,621) | 1:628:A:LEU:HD11 | 1:628:A:LEU:HA   | 11       | 1.27          |
| (1,621) | 1:628:A:LEU:HD11 | 1:628:A:LEU:HA   | 12       | 1.27          |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD11 | 6        | 1.27          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 7        | 1.27          |
| (1,286) | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 14       | 1.27          |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 1        | 1.27          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,142) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HE1  | 3        | 1.27          |
| (1,142) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HE2  | 3        | 1.27          |
| (1,87)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 9        | 1.27          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 4        | 1.26          |
| (1,742) | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 15       | 1.26          |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 13       | 1.26          |
| (1,621) | 1:628:A:LEU:HD11 | 1:628:A:LEU:HA   | 20       | 1.26          |
| (1,581) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 16       | 1.26          |
| (1,523) | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD2  | 7        | 1.26          |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD21 | 18       | 1.26          |
| (1,303) | 1:664:A:LEU:HD11 | 1:664:A:LEU:HA   | 3        | 1.26          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 2        | 1.26          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 9        | 1.26          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 14       | 1.26          |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 15       | 1.25          |
| (1,742) | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 19       | 1.25          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD13 | 3        | 1.25          |
| (1,406) | 1:635:A:VAL:HG21 | 1:656:A:LYS:HG2  | 9        | 1.25          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 9        | 1.25          |
| (1,32)  | 1:648:A:GLU:HB2  | 1:643:A:ALA:HB2  | 2        | 1.25          |
| (1,742) | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 7        | 1.24          |
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD12 | 17       | 1.24          |
| (1,594) | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG12 | 18       | 1.24          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 14       | 1.24          |
| (1,484) | 1:607:A:LEU:HD22 | 1:653:A:LEU:HB2  | 1        | 1.24          |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE3  | 8        | 1.24          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD11 | 18       | 1.24          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 6        | 1.24          |
| (1,286) | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 8        | 1.24          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 9        | 1.23          |
| (2,95)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HB3  | 6        | 1.23          |
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 12       | 1.23          |
| (1,793) | 1:618:A:ALA:H    | 1:617:A:PRO:HG2  | 10       | 1.23          |
| (1,742) | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 4        | 1.23          |
| (1,742) | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 6        | 1.23          |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 7        | 1.23          |
| (1,636) | 1:639:A:MET:HE3  | 1:639:A:MET:HA   | 15       | 1.23          |
| (1,603) | 1:599:A:LEU:HD12 | 1:595:A:VAL:HG11 | 2        | 1.23          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 16       | 1.23          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 17       | 1.23          |
| (1,583) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD12 | 16       | 1.23          |
| (1,436) | 1:653:A:LEU:HA   | 1:639:A:MET:HE3  | 18       | 1.23          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB2  | 14       | 1.23          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 3        | 1.23          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 10       | 1.22          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 10       | 1.22          |
| (1,636) | 1:639:A:MET:HE2  | 1:639:A:MET:HA   | 13       | 1.22          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 13       | 1.22          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 19       | 1.22          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 20       | 1.22          |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD11 | 3        | 1.22          |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD11 | 3        | 1.22          |
| (1,480) | 1:653:A:LEU:HD21 | 1:636:A:GLU:HA   | 15       | 1.22          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE3  | 8        | 1.22          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE1  | 12       | 1.22          |
| (1,423) | 1:629:A:VAL:HG12 | 1:626:A:GLU:HG2  | 5        | 1.22          |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD11 | 4        | 1.22          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 9        | 1.22          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 12       | 1.22          |
| (1,5)   | 1:608:A:VAL:HG21 | 1:625:A:MET:HE3  | 4        | 1.22          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 8        | 1.21          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 16       | 1.21          |
| (1,793) | 1:618:A:ALA:H    | 1:617:A:PRO:HG2  | 15       | 1.21          |
| (1,639) | 1:652:A:LEU:HD21 | 1:642:A:SER:HB2  | 6        | 1.21          |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD22 | 7        | 1.21          |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD13 | 12       | 1.21          |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD13 | 12       | 1.21          |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD22 | 1        | 1.21          |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 13       | 1.21          |
| (1,258) | 1:656:A:LYS:HA   | 1:659:A:LYS:HB3  | 19       | 1.21          |
| (1,210) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD21 | 6        | 1.21          |
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD1  | 5        | 1.21          |
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD2  | 5        | 1.21          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 10       | 1.2           |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 14       | 1.2           |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 14       | 1.2           |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 14       | 1.2           |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 3        | 1.2           |
| (1,942) | 1:664:A:LEU:H    | 1:664:A:LEU:HD12 | 3        | 1.2           |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD23 | 5        | 1.2           |
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 18       | 1.2           |
| (1,812) | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 17       | 1.2           |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 5        | 1.2           |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 9        | 1.2           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 20       | 1.2           |
| (1,621) | 1:628:A:LEU:HD12 | 1:628:A:LEU:HA   | 15       | 1.2           |
| (1,495) | 1:653:A:LEU:HD13 | 1:603:A:LEU:HD13 | 14       | 1.2           |
| (1,397) | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB1  | 20       | 1.2           |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD12 | 19       | 1.2           |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 4        | 1.2           |
| (1,297) | 1:633:A:LYS:HD3  | 1:633:A:LYS:HA   | 18       | 1.2           |
| (1,258) | 1:656:A:LYS:HA   | 1:659:A:LYS:HB3  | 6        | 1.2           |
| (1,258) | 1:656:A:LYS:HA   | 1:659:A:LYS:HB3  | 16       | 1.2           |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 20       | 1.19          |
| (1,812) | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 1        | 1.19          |
| (1,793) | 1:618:A:ALA:H    | 1:617:A:PRO:HG2  | 1        | 1.19          |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 3        | 1.19          |
| (1,654) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 8        | 1.19          |
| (1,643) | 1:608:A:VAL:HG23 | 1:608:A:VAL:HA   | 7        | 1.19          |
| (1,643) | 1:608:A:VAL:HG21 | 1:608:A:VAL:HA   | 17       | 1.19          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 15       | 1.19          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE1  | 11       | 1.19          |
| (1,258) | 1:656:A:LYS:HA   | 1:659:A:LYS:HB3  | 10       | 1.19          |
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD11 | 5        | 1.18          |
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD12 | 9        | 1.18          |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD11 | 5        | 1.18          |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD11 | 5        | 1.18          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 1        | 1.18          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 8        | 1.18          |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 17       | 1.18          |
| (1,348) | 1:606:A:LYS:HD2  | 1:657:A:ILE:HD11 | 6        | 1.18          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 19       | 1.18          |
| (1,258) | 1:656:A:LYS:HA   | 1:659:A:LYS:HB3  | 3        | 1.18          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE1  | 1        | 1.18          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE2  | 1        | 1.18          |
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD1  | 14       | 1.18          |
| (1,116) | 1:653:A:LEU:HD13 | 1:650:A:TYR:HD2  | 14       | 1.18          |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 8        | 1.18          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 20       | 1.18          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE1  | 19       | 1.17          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE2  | 19       | 1.17          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE1  | 19       | 1.17          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE2  | 19       | 1.17          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE1  | 19       | 1.17          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE2  | 19       | 1.17          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 3        | 1.17          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 3        | 1.17          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 3        | 1.17          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 3        | 1.17          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 3        | 1.17          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 3        | 1.17          |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD22 | 16       | 1.17          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 6        | 1.17          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 6        | 1.17          |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 7        | 1.17          |
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD11 | 16       | 1.17          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD12 | 6        | 1.17          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD12 | 6        | 1.17          |
| (1,623) | 1:631:A:TYR:HB2  | 1:628:A:LEU:HD12 | 6        | 1.17          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 1        | 1.17          |
| (1,484) | 1:607:A:LEU:HD23 | 1:653:A:LEU:HB2  | 7        | 1.17          |
| (1,470) | 1:635:A:VAL:HG12 | 1:639:A:MET:HE2  | 7        | 1.17          |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 13       | 1.17          |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 9        | 1.17          |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD11 | 13       | 1.17          |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 7        | 1.16          |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD22 | 19       | 1.16          |
| (1,857) | 1:636:A:GLU:H    | 1:635:A:VAL:HG21 | 15       | 1.16          |
| (1,654) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 1        | 1.16          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 10       | 1.16          |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD12 | 10       | 1.16          |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD12 | 10       | 1.16          |
| (1,581) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 6        | 1.16          |
| (1,581) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 13       | 1.16          |
| (1,495) | 1:653:A:LEU:HD11 | 1:603:A:LEU:HD13 | 4        | 1.16          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 12       | 1.16          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 5        | 1.16          |
| (1,286) | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 11       | 1.16          |
| (1,270) | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 2        | 1.16          |
| (1,118) | 1:653:A:LEU:HB3  | 1:650:A:TYR:HA   | 6        | 1.16          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 1        | 1.16          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 16       | 1.16          |
| (2,136) | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 12       | 1.15          |
| (2,136) | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 13       | 1.15          |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD23 | 4        | 1.15          |
| (1,686) | 1:601:A:SER:H    | 1:600:A:ARG:HG2  | 14       | 1.15          |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG23 | 13       | 1.15          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 1        | 1.15          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 7        | 1.15          |
| (1,581) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 2        | 1.15          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 2        | 1.15          |
| (1,484) | 1:607:A:LEU:HD22 | 1:653:A:LEU:HB2  | 6        | 1.15          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD11 | 2        | 1.15          |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 4        | 1.15          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 9        | 1.15          |
| (2,275) | 2:546:B:LEU:H    | 2:545:B:LEU:HD11 | 3        | 1.14          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD1  | 12       | 1.14          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD2  | 12       | 1.14          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD1  | 12       | 1.14          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD2  | 12       | 1.14          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD1  | 12       | 1.14          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD2  | 12       | 1.14          |
| (1,944) | 1:666:A:GLU:H    | 1:666:A:GLU:HG2  | 3        | 1.14          |
| (1,944) | 1:666:A:GLU:H    | 1:666:A:GLU:HG2  | 7        | 1.14          |
| (1,944) | 1:666:A:GLU:H    | 1:666:A:GLU:HG2  | 15       | 1.14          |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD22 | 8        | 1.14          |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD23 | 13       | 1.14          |
| (1,605) | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD23 | 14       | 1.14          |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 11       | 1.14          |
| (1,581) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 8        | 1.14          |
| (1,499) | 1:639:A:MET:HG3  | 1:652:A:LEU:HD22 | 1        | 1.14          |
| (1,470) | 1:635:A:VAL:HG11 | 1:639:A:MET:HE1  | 2        | 1.14          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE3  | 13       | 1.14          |
| (1,401) | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB1  | 10       | 1.14          |
| (1,286) | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 12       | 1.14          |
| (1,286) | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 13       | 1.14          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD1  | 8        | 1.14          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD2  | 8        | 1.14          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 7        | 1.14          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 17       | 1.13          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 17       | 1.13          |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 19       | 1.13          |
| (1,654) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 12       | 1.13          |
| (1,450) | 1:665:A:GLU:HA   | 1:665:A:GLU:HG2  | 15       | 1.13          |
| (1,435) | 1:653:A:LEU:HD12 | 1:639:A:MET:HE3  | 13       | 1.13          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 20       | 1.13          |
| (1,133) | 1:640:A:TYR:HA   | 1:649:A:TYR:HD1  | 9        | 1.13          |
| (1,133) | 1:640:A:TYR:HA   | 1:649:A:TYR:HD2  | 9        | 1.13          |
| (1,32)  | 1:648:A:GLU:HB2  | 1:643:A:ALA:HB1  | 4        | 1.13          |
| (1,992) | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 11       | 1.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,991)  | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 11       | 1.12          |
| (1,902)  | 1:653:A:LEU:H    | 1:652:A:LEU:HD21 | 1        | 1.12          |
| (1,902)  | 1:653:A:LEU:H    | 1:652:A:LEU:HD23 | 15       | 1.12          |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 20       | 1.12          |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 20       | 1.12          |
| (1,812)  | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 10       | 1.12          |
| (1,654)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 14       | 1.12          |
| (1,650)  | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 6        | 1.12          |
| (1,650)  | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 15       | 1.12          |
| (1,608)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD21 | 13       | 1.12          |
| (1,608)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD23 | 16       | 1.12          |
| (1,593)  | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 12       | 1.12          |
| (1,584)  | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD11 | 20       | 1.12          |
| (1,584)  | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD11 | 20       | 1.12          |
| (1,581)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 20       | 1.12          |
| (1,397)  | 1:611:A:ILE:HG12 | 1:610:A:ALA:HB2  | 3        | 1.12          |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 1        | 1.12          |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 3        | 1.12          |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 4        | 1.12          |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 5        | 1.12          |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 7        | 1.12          |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 17       | 1.12          |
| (1,117)  | 1:653:A:LEU:HD21 | 1:650:A:TYR:HD1  | 19       | 1.12          |
| (1,117)  | 1:653:A:LEU:HD21 | 1:650:A:TYR:HD2  | 19       | 1.12          |
| (1,87)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 1        | 1.12          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 9        | 1.11          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 20       | 1.11          |
| (1,944)  | 1:666:A:GLU:H    | 1:666:A:GLU:HG2  | 20       | 1.11          |
| (1,639)  | 1:652:A:LEU:HD23 | 1:642:A:SER:HB2  | 11       | 1.11          |
| (1,584)  | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD12 | 17       | 1.11          |
| (1,584)  | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD12 | 17       | 1.11          |
| (1,581)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 1        | 1.11          |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 10       | 1.11          |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 15       | 1.11          |
| (1,70)   | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 3        | 1.11          |
| (3,21)   | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD1  | 19       | 1.1           |
| (3,21)   | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD2  | 19       | 1.1           |
| (3,21)   | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD1  | 19       | 1.1           |
| (3,21)   | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD2  | 19       | 1.1           |
| (3,21)   | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD1  | 19       | 1.1           |
| (3,21)   | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD2  | 19       | 1.1           |
| (1,989)  | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD21 | 7        | 1.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,989)  | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD22 | 7        | 1.1           |
| (1,989)  | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD23 | 7        | 1.1           |
| (1,989)  | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD21 | 7        | 1.1           |
| (1,989)  | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD22 | 7        | 1.1           |
| (1,989)  | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD23 | 7        | 1.1           |
| (1,902)  | 1:653:A:LEU:H    | 1:652:A:LEU:HD22 | 6        | 1.1           |
| (1,902)  | 1:653:A:LEU:H    | 1:652:A:LEU:HD21 | 11       | 1.1           |
| (1,902)  | 1:653:A:LEU:H    | 1:652:A:LEU:HD22 | 12       | 1.1           |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 11       | 1.1           |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 11       | 1.1           |
| (1,636)  | 1:639:A:MET:HE1  | 1:639:A:MET:HA   | 19       | 1.1           |
| (1,600)  | 1:646:A:ARG:HA   | 1:595:A:VAL:HG23 | 5        | 1.1           |
| (1,495)  | 1:653:A:LEU:HD12 | 1:603:A:LEU:HD12 | 13       | 1.1           |
| (1,495)  | 1:653:A:LEU:HD12 | 1:603:A:LEU:HD13 | 17       | 1.1           |
| (1,374)  | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG13 | 4        | 1.1           |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 16       | 1.1           |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 19       | 1.1           |
| (1,263)  | 1:607:A:LEU:HD21 | 1:632:A:ALA:HB2  | 5        | 1.1           |
| (1,39)   | 1:662:A:LYS:HG2  | 1:659:A:LYS:HD3  | 11       | 1.1           |
| (1,32)   | 1:648:A:GLU:HB2  | 1:643:A:ALA:HB1  | 7        | 1.1           |
| (3,9)    | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 12       | 1.09          |
| (3,9)    | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 12       | 1.09          |
| (3,9)    | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 12       | 1.09          |
| (3,9)    | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 12       | 1.09          |
| (3,9)    | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 12       | 1.09          |
| (3,9)    | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 12       | 1.09          |
| (3,9)    | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 12       | 1.09          |
| (3,9)    | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 12       | 1.09          |
| (3,9)    | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 12       | 1.09          |
| (2,95)   | 2:537:B:ILE:HB   | 2:534:B:PHE:HB3  | 16       | 1.09          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 6        | 1.09          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 6        | 1.09          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 6        | 1.09          |
| (1,951)  | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 8        | 1.09          |
| (1,933)  | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 11       | 1.09          |
| (1,715)  | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 19       | 1.09          |
| (1,695)  | 1:641:A:GLU:H    | 1:641:A:GLU:HG2  | 11       | 1.09          |
| (1,650)  | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 20       | 1.09          |
| (1,581)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 12       | 1.09          |
| (1,485)  | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 10       | 1.09          |
| (1,485)  | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 11       | 1.09          |
| (1,484)  | 1:607:A:LEU:HD23 | 1:653:A:LEU:HB2  | 15       | 1.09          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,406)  | 1:635:A:VAL:HG22 | 1:656:A:LYS:HG2  | 13       | 1.09          |
| (1,366)  | 1:639:A:MET:HE3  | 1:653:A:LEU:HD21 | 10       | 1.09          |
| (1,366)  | 1:639:A:MET:HE2  | 1:653:A:LEU:HD22 | 20       | 1.09          |
| (1,270)  | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 4        | 1.09          |
| (1,258)  | 1:656:A:LYS:HA   | 1:659:A:LYS:HB3  | 12       | 1.09          |
| (1,143)  | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 16       | 1.09          |
| (1,143)  | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 16       | 1.09          |
| (2,111)  | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD11 | 20       | 1.08          |
| (2,111)  | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD12 | 20       | 1.08          |
| (2,111)  | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD13 | 20       | 1.08          |
| (2,111)  | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD11 | 20       | 1.08          |
| (2,111)  | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD12 | 20       | 1.08          |
| (2,111)  | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD13 | 20       | 1.08          |
| (1,983)  | 1:607:A:LEU:H    | 1:607:A:LEU:HD23 | 5        | 1.08          |
| (1,983)  | 1:607:A:LEU:H    | 1:607:A:LEU:HD21 | 13       | 1.08          |
| (1,902)  | 1:653:A:LEU:H    | 1:652:A:LEU:HD21 | 7        | 1.08          |
| (1,650)  | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 14       | 1.08          |
| (1,650)  | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 17       | 1.08          |
| (1,639)  | 1:652:A:LEU:HD23 | 1:642:A:SER:HB2  | 7        | 1.08          |
| (1,613)  | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 13       | 1.08          |
| (1,610)  | 1:599:A:LEU:HD23 | 1:603:A:LEU:HD22 | 12       | 1.08          |
| (1,509)  | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 12       | 1.08          |
| (1,485)  | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 7        | 1.08          |
| (1,345)  | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD11 | 5        | 1.08          |
| (1,295)  | 1:633:A:LYS:HA   | 1:604:A:VAL:HG12 | 19       | 1.08          |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 18       | 1.08          |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 20       | 1.08          |
| (1,92)   | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 1        | 1.08          |
| (1,87)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 7        | 1.08          |
| (1,86)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 11       | 1.08          |
| (1,6)    | 1:608:A:VAL:HG13 | 1:625:A:MET:HE1  | 18       | 1.08          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 16       | 1.07          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG11 | 12       | 1.07          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG12 | 12       | 1.07          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG13 | 12       | 1.07          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG11 | 12       | 1.07          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG12 | 12       | 1.07          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG13 | 12       | 1.07          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG11 | 12       | 1.07          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG12 | 12       | 1.07          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG13 | 12       | 1.07          |
| (1,902)  | 1:653:A:LEU:H    | 1:652:A:LEU:HD21 | 9        | 1.07          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 1        | 1.07          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 3        | 1.07          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 3        | 1.07          |
| (1,857) | 1:636:A:GLU:H    | 1:635:A:VAL:HG22 | 14       | 1.07          |
| (1,812) | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 18       | 1.07          |
| (1,650) | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 8        | 1.07          |
| (1,650) | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 9        | 1.07          |
| (1,650) | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 18       | 1.07          |
| (1,594) | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG13 | 19       | 1.07          |
| (1,581) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 5        | 1.07          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 7        | 1.07          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD12 | 16       | 1.07          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 4        | 1.07          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 13       | 1.07          |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 20       | 1.07          |
| (1,167) | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 3        | 1.07          |
| (1,87)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 10       | 1.07          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 17       | 1.06          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 17       | 1.06          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 17       | 1.06          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 17       | 1.06          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 17       | 1.06          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 17       | 1.06          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 17       | 1.06          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 17       | 1.06          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 17       | 1.06          |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD21 | 14       | 1.06          |
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 17       | 1.06          |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 15       | 1.06          |
| (1,650) | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 12       | 1.06          |
| (1,636) | 1:639:A:MET:HE2  | 1:639:A:MET:HA   | 11       | 1.06          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD12 | 8        | 1.06          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD12 | 8        | 1.06          |
| (1,548) | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 20       | 1.06          |
| (1,424) | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 11       | 1.06          |
| (1,214) | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD12 | 11       | 1.06          |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 5        | 1.06          |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 19       | 1.06          |
| (1,167) | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 7        | 1.06          |
| (1,167) | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 11       | 1.06          |
| (1,87)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 2        | 1.06          |
| (1,32)  | 1:648:A:GLU:HB2  | 1:643:A:ALA:HB2  | 16       | 1.06          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,5)    | 1:608:A:VAL:HG22 | 1:625:A:MET:HE2  | 10       | 1.06          |
| (2,136)  | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 9        | 1.05          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 10       | 1.05          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 10       | 1.05          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 10       | 1.05          |
| (1,902)  | 1:653:A:LEU:H    | 1:652:A:LEU:HD22 | 20       | 1.05          |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 5        | 1.05          |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 5        | 1.05          |
| (1,711)  | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 7        | 1.05          |
| (1,699)  | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 18       | 1.05          |
| (1,639)  | 1:652:A:LEU:HD22 | 1:642:A:SER:HB2  | 13       | 1.05          |
| (1,424)  | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 8        | 1.05          |
| (1,366)  | 1:639:A:MET:HE1  | 1:653:A:LEU:HD21 | 11       | 1.05          |
| (1,258)  | 1:656:A:LYS:HA   | 1:659:A:LYS:HB3  | 2        | 1.05          |
| (1,214)  | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD11 | 2        | 1.05          |
| (1,214)  | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD12 | 8        | 1.05          |
| (1,214)  | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD11 | 15       | 1.05          |
| (1,214)  | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD13 | 16       | 1.05          |
| (1,214)  | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD13 | 20       | 1.05          |
| (1,194)  | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 3        | 1.05          |
| (1,171)  | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 17       | 1.05          |
| (1,167)  | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 6        | 1.05          |
| (1,167)  | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 8        | 1.05          |
| (1,167)  | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 10       | 1.05          |
| (1,167)  | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 20       | 1.05          |
| (1,143)  | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 3        | 1.05          |
| (1,143)  | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 3        | 1.05          |
| (1,117)  | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD1  | 16       | 1.05          |
| (1,117)  | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD2  | 16       | 1.05          |
| (1,92)   | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 11       | 1.05          |
| (1,87)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 18       | 1.05          |
| (1,71)   | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 11       | 1.05          |
| (2,136)  | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 19       | 1.04          |
| (1,933)  | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 1        | 1.04          |
| (1,933)  | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 7        | 1.04          |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 13       | 1.04          |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 13       | 1.04          |
| (1,802)  | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 12       | 1.04          |
| (1,787)  | 1:616:A:ASP:H    | 1:614:A:THR:HG21 | 13       | 1.04          |
| (1,581)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 4        | 1.04          |
| (1,548)  | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 9        | 1.04          |
| (1,423)  | 1:629:A:VAL:HG12 | 1:626:A:GLU:HG2  | 14       | 1.04          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 6        | 1.04          |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 9        | 1.04          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 17       | 1.04          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 20       | 1.03          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 6        | 1.03          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 6        | 1.03          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 6        | 1.03          |
| (1,951) | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 14       | 1.03          |
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 8        | 1.03          |
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 11       | 1.03          |
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 14       | 1.03          |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 14       | 1.03          |
| (1,639) | 1:652:A:LEU:HD21 | 1:642:A:SER:HB2  | 2        | 1.03          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD22 | 4        | 1.03          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 10       | 1.03          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 12       | 1.03          |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 7        | 1.03          |
| (1,92)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HE3  | 13       | 1.03          |
| (1,87)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 11       | 1.03          |
| (1,86)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE2  | 12       | 1.03          |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD21 | 3        | 1.02          |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD21 | 18       | 1.02          |
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 2        | 1.02          |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 3        | 1.02          |
| (1,772) | 1:608:A:VAL:H    | 1:608:A:VAL:HG23 | 1        | 1.02          |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 10       | 1.02          |
| (1,639) | 1:652:A:LEU:HD23 | 1:642:A:SER:HB2  | 1        | 1.02          |
| (1,571) | 1:591:A:TRP:HD1  | 1:589:A:LYS:HA   | 2        | 1.02          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 1        | 1.02          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 10       | 1.02          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 15       | 1.02          |
| (1,258) | 1:656:A:LYS:HA   | 1:659:A:LYS:HB3  | 18       | 1.02          |
| (1,229) | 1:636:A:GLU:HG2  | 1:604:A:VAL:HG22 | 3        | 1.02          |
| (1,214) | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD13 | 9        | 1.02          |
| (1,167) | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 5        | 1.02          |
| (1,106) | 1:650:A:TYR:HA   | 1:650:A:TYR:HD1  | 2        | 1.02          |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD11 | 1        | 1.02          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE1  | 8        | 1.01          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE2  | 8        | 1.01          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE1  | 8        | 1.01          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE2  | 8        | 1.01          |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE1  | 8        | 1.01          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE2  | 8        | 1.01          |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD21 | 7        | 1.01          |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD22 | 7        | 1.01          |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD23 | 7        | 1.01          |
| (2,136) | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 2        | 1.01          |
| (2,136) | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 5        | 1.01          |
| (2,136) | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 15       | 1.01          |
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 20       | 1.01          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 9        | 1.01          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 9        | 1.01          |
| (1,853) | 1:635:A:VAL:H    | 1:635:A:VAL:HG13 | 6        | 1.01          |
| (1,812) | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 5        | 1.01          |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 8        | 1.01          |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 19       | 1.01          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD13 | 7        | 1.01          |
| (1,583) | 1:603:A:LEU:HD13 | 1:599:A:LEU:HD13 | 1        | 1.01          |
| (1,496) | 1:599:A:LEU:HD11 | 1:603:A:LEU:HD21 | 14       | 1.01          |
| (1,484) | 1:607:A:LEU:HD21 | 1:653:A:LEU:HB2  | 16       | 1.01          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 18       | 1.01          |
| (1,411) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HB2  | 2        | 1.01          |
| (1,366) | 1:639:A:MET:HE1  | 1:653:A:LEU:HD21 | 14       | 1.01          |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG22 | 19       | 1.01          |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 11       | 1.01          |
| (1,167) | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 4        | 1.01          |
| (1,142) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE1  | 12       | 1.01          |
| (1,142) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE2  | 12       | 1.01          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 20       | 1.01          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 4        | 1.0           |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 4        | 1.0           |
| (3,21)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD1  | 2        | 1.0           |
| (3,21)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD2  | 2        | 1.0           |
| (3,21)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD1  | 2        | 1.0           |
| (3,21)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD2  | 2        | 1.0           |
| (3,21)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD1  | 2        | 1.0           |
| (3,21)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD2  | 2        | 1.0           |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 3        | 1.0           |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 3        | 1.0           |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 3        | 1.0           |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 3        | 1.0           |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 3        | 1.0           |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 3        | 1.0           |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 1        | 1.0           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 18       | 1.0           |
| (2,136) | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 14       | 1.0           |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD23 | 9        | 1.0           |
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 3        | 1.0           |
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 7        | 1.0           |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 14       | 1.0           |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 14       | 1.0           |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 18       | 1.0           |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 18       | 1.0           |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 1        | 1.0           |
| (1,639) | 1:652:A:LEU:HD22 | 1:642:A:SER:HB2  | 4        | 1.0           |
| (1,639) | 1:652:A:LEU:HD23 | 1:642:A:SER:HB2  | 17       | 1.0           |
| (1,610) | 1:599:A:LEU:HD21 | 1:603:A:LEU:HD21 | 15       | 1.0           |
| (1,598) | 1:595:A:VAL:HG23 | 1:592:A:HIS:HA   | 14       | 1.0           |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE3  | 18       | 1.0           |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG11 | 5        | 1.0           |
| (1,366) | 1:639:A:MET:HE2  | 1:653:A:LEU:HD23 | 2        | 1.0           |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 11       | 1.0           |
| (1,270) | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 10       | 1.0           |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 6        | 1.0           |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 14       | 1.0           |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE1  | 5        | 0.99          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE2  | 5        | 0.99          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE1  | 5        | 0.99          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE2  | 5        | 0.99          |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE1  | 5        | 0.99          |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE2  | 5        | 0.99          |
| (2,252) | 2:535:B:SER:H    | 2:534:B:PHE:HD1  | 6        | 0.99          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 5        | 0.99          |
| (2,136) | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 7        | 0.99          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD11 | 11       | 0.99          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD12 | 11       | 0.99          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD13 | 11       | 0.99          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD11 | 11       | 0.99          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD12 | 11       | 0.99          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD13 | 11       | 0.99          |
| (1,992) | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 5        | 0.99          |
| (1,991) | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 5        | 0.99          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 5        | 0.99          |
| (1,857) | 1:636:A:GLU:H    | 1:635:A:VAL:HG21 | 1        | 0.99          |
| (1,857) | 1:636:A:GLU:H    | 1:635:A:VAL:HG22 | 9        | 0.99          |
| (1,787) | 1:616:A:ASP:H    | 1:614:A:THR:HG22 | 19       | 0.99          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD13 | 15       | 0.99          |
| (1,639) | 1:652:A:LEU:HD23 | 1:642:A:SER:HB2  | 9        | 0.99          |
| (1,636) | 1:639:A:MET:HE1  | 1:639:A:MET:HA   | 8        | 0.99          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD12 | 1        | 0.99          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD12 | 1        | 0.99          |
| (1,617) | 1:653:A:LEU:HG   | 1:639:A:MET:HG3  | 14       | 0.99          |
| (1,596) | 1:632:A:ALA:HB2  | 1:635:A:VAL:HG22 | 12       | 0.99          |
| (1,583) | 1:603:A:LEU:HD11 | 1:599:A:LEU:HD13 | 13       | 0.99          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 15       | 0.99          |
| (1,435) | 1:653:A:LEU:HD11 | 1:639:A:MET:HE3  | 5        | 0.99          |
| (1,432) | 1:653:A:LEU:HG   | 1:639:A:MET:HE2  | 15       | 0.99          |
| (1,302) | 1:614:A:THR:HG23 | 1:617:A:PRO:HA   | 7        | 0.99          |
| (1,270) | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 8        | 0.99          |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 15       | 0.99          |
| (1,87)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 19       | 0.99          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 4        | 0.99          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 11       | 0.99          |
| (2,136) | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 11       | 0.98          |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD21 | 4        | 0.98          |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD21 | 17       | 0.98          |
| (1,853) | 1:635:A:VAL:H    | 1:635:A:VAL:HG11 | 2        | 0.98          |
| (1,853) | 1:635:A:VAL:H    | 1:635:A:VAL:HG12 | 3        | 0.98          |
| (1,812) | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 20       | 0.98          |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 7        | 0.98          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD1  | 12       | 0.98          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD2  | 12       | 0.98          |
| (1,596) | 1:632:A:ALA:HB3  | 1:635:A:VAL:HG22 | 5        | 0.98          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 3        | 0.98          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 12       | 0.98          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 19       | 0.98          |
| (1,411) | 1:629:A:VAL:HG11 | 1:630:A:ALA:HB2  | 3        | 0.98          |
| (1,270) | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 17       | 0.98          |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG23 | 5        | 0.98          |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 2        | 0.98          |
| (1,167) | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 9        | 0.98          |
| (1,167) | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 16       | 0.98          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 16       | 0.97          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 16       | 0.97          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 16       | 0.97          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 16       | 0.97          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 16       | 0.97          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 16       | 0.97          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD21 | 20       | 0.97          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD22 | 20       | 0.97          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD23 | 20       | 0.97          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD21 | 20       | 0.97          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD22 | 20       | 0.97          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD23 | 20       | 0.97          |
| (2,136) | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 17       | 0.97          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD11 | 6        | 0.97          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD12 | 6        | 0.97          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD13 | 6        | 0.97          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD11 | 6        | 0.97          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD12 | 6        | 0.97          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD13 | 6        | 0.97          |
| (1,992) | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 19       | 0.97          |
| (1,991) | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 19       | 0.97          |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD23 | 10       | 0.97          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 8        | 0.97          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 8        | 0.97          |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 11       | 0.97          |
| (1,583) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD11 | 10       | 0.97          |
| (1,484) | 1:607:A:LEU:HD23 | 1:653:A:LEU:HB2  | 20       | 0.97          |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD21 | 1        | 0.97          |
| (1,415) | 1:620:A:LEU:HD21 | 1:625:A:MET:HG2  | 10       | 0.97          |
| (1,270) | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 6        | 0.97          |
| (1,270) | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 13       | 0.97          |
| (1,268) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HB3  | 11       | 0.97          |
| (1,268) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HB3  | 15       | 0.97          |
| (1,258) | 1:656:A:LYS:HA   | 1:659:A:LYS:HB3  | 9        | 0.97          |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE1  | 15       | 0.97          |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE2  | 15       | 0.97          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD12 | 10       | 0.97          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD12 | 10       | 0.97          |
| (1,118) | 1:653:A:LEU:HB3  | 1:650:A:TYR:HA   | 9        | 0.97          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 7        | 0.97          |
| (2,136) | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 1        | 0.96          |
| (2,136) | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 8        | 0.96          |
| (2,104) | 2:539:B:ASP:HB3  | 2:536:B:SER:HB2  | 2        | 0.96          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 16       | 0.96          |
| (1,902) | 1:653:A:LEU:H    | 1:652:A:LEU:HD22 | 2        | 0.96          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 7        | 0.96          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 7        | 0.96          |
| (1,857) | 1:636:A:GLU:H    | 1:635:A:VAL:HG21 | 20       | 0.96          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,853)  | 1:635:A:VAL:H    | 1:635:A:VAL:HG12 | 11       | 0.96          |
| (1,787)  | 1:616:A:ASP:H    | 1:614:A:THR:HG23 | 18       | 0.96          |
| (1,699)  | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 13       | 0.96          |
| (1,699)  | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 17       | 0.96          |
| (1,613)  | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 20       | 0.96          |
| (1,581)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 19       | 0.96          |
| (1,452)  | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 16       | 0.96          |
| (1,441)  | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD23 | 3        | 0.96          |
| (1,441)  | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD21 | 8        | 0.96          |
| (1,374)  | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG12 | 1        | 0.96          |
| (1,326)  | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 2        | 0.96          |
| (1,167)  | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 19       | 0.96          |
| (1,986)  | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 4        | 0.95          |
| (1,939)  | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 9        | 0.95          |
| (1,900)  | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 16       | 0.95          |
| (1,717)  | 1:610:A:ALA:H    | 1:657:A:ILE:HD12 | 14       | 0.95          |
| (1,699)  | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 16       | 0.95          |
| (1,584)  | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD13 | 7        | 0.95          |
| (1,584)  | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD13 | 7        | 0.95          |
| (1,581)  | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 10       | 0.95          |
| (1,536)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD21 | 16       | 0.95          |
| (1,480)  | 1:653:A:LEU:HD22 | 1:636:A:GLU:HA   | 17       | 0.95          |
| (1,462)  | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 13       | 0.95          |
| (1,441)  | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD23 | 6        | 0.95          |
| (1,441)  | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD23 | 9        | 0.95          |
| (1,326)  | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 6        | 0.95          |
| (1,270)  | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 3        | 0.95          |
| (1,270)  | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 9        | 0.95          |
| (1,270)  | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 14       | 0.95          |
| (1,194)  | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 8        | 0.95          |
| (1,185)  | 1:621:A:LYS:HD2  | 1:621:A:LYS:HB2  | 20       | 0.95          |
| (1,167)  | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 18       | 0.95          |
| (3,29)   | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 14       | 0.94          |
| (3,29)   | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 14       | 0.94          |
| (3,19)   | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 20       | 0.94          |
| (3,19)   | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 20       | 0.94          |
| (3,19)   | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 20       | 0.94          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 20       | 0.94          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 20       | 0.94          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 20       | 0.94          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 11       | 0.94          |
| (1,983)  | 1:607:A:LEU:H    | 1:607:A:LEU:HD22 | 11       | 0.94          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD22 | 20       | 0.94          |
| (1,933) | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 12       | 0.94          |
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 15       | 0.94          |
| (1,900) | 1:653:A:LEU:H    | 1:653:A:LEU:HG   | 19       | 0.94          |
| (1,898) | 1:653:A:LEU:H    | 1:655:A:GLU:HG2  | 14       | 0.94          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 1        | 0.94          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 1        | 0.94          |
| (1,853) | 1:635:A:VAL:H    | 1:635:A:VAL:HG11 | 8        | 0.94          |
| (1,853) | 1:635:A:VAL:H    | 1:635:A:VAL:HG13 | 16       | 0.94          |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 16       | 0.94          |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 8        | 0.94          |
| (1,654) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 19       | 0.94          |
| (1,639) | 1:652:A:LEU:HD21 | 1:642:A:SER:HB2  | 8        | 0.94          |
| (1,613) | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 11       | 0.94          |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD13 | 1        | 0.94          |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD13 | 1        | 0.94          |
| (1,571) | 1:591:A:TRP:HD1  | 1:589:A:LYS:HA   | 10       | 0.94          |
| (1,548) | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 8        | 0.94          |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD21 | 4        | 0.94          |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD21 | 5        | 0.94          |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD21 | 10       | 0.94          |
| (1,411) | 1:629:A:VAL:HG12 | 1:630:A:ALA:HB3  | 15       | 0.94          |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG12 | 9        | 0.94          |
| (1,362) | 1:608:A:VAL:HG13 | 1:608:A:VAL:HA   | 1        | 0.94          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 8        | 0.94          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 4        | 0.94          |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 17       | 0.94          |
| (1,185) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HB2  | 11       | 0.94          |
| (1,185) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HB2  | 14       | 0.94          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 5        | 0.93          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 5        | 0.93          |
| (2,252) | 2:535:B:SER:H    | 2:534:B:PHE:HD1  | 20       | 0.93          |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD21 | 2        | 0.93          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 2        | 0.93          |
| (1,933) | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 3        | 0.93          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 16       | 0.93          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 16       | 0.93          |
| (1,812) | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 11       | 0.93          |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 5        | 0.93          |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 9        | 0.93          |
| (1,654) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 7        | 0.93          |
| (1,654) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 9        | 0.93          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD12 | 18       | 0.93          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD12 | 18       | 0.93          |
| (1,571) | 1:591:A:TRP:HD1  | 1:589:A:LYS:HA   | 18       | 0.93          |
| (1,548) | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 2        | 0.93          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 2        | 0.93          |
| (1,464) | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 20       | 0.93          |
| (1,452) | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 9        | 0.93          |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD23 | 20       | 0.93          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 16       | 0.93          |
| (1,268) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HB3  | 20       | 0.93          |
| (1,185) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HB2  | 10       | 0.93          |
| (1,167) | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 12       | 0.93          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD21 | 3        | 0.92          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD22 | 3        | 0.92          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD23 | 3        | 0.92          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD21 | 3        | 0.92          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD22 | 3        | 0.92          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD23 | 3        | 0.92          |
| (2,252) | 2:535:B:SER:H    | 2:534:B:PHE:HD1  | 2        | 0.92          |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD21 | 8        | 0.92          |
| (1,971) | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 6        | 0.92          |
| (1,933) | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 4        | 0.92          |
| (1,933) | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 6        | 0.92          |
| (1,933) | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 10       | 0.92          |
| (1,812) | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 7        | 0.92          |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 1        | 0.92          |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 9        | 0.92          |
| (1,654) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 6        | 0.92          |
| (1,639) | 1:652:A:LEU:HD21 | 1:642:A:SER:HB2  | 16       | 0.92          |
| (1,613) | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 15       | 0.92          |
| (1,613) | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 17       | 0.92          |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD13 | 16       | 0.92          |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD13 | 16       | 0.92          |
| (1,581) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 7        | 0.92          |
| (1,484) | 1:607:A:LEU:HD22 | 1:653:A:LEU:HB2  | 2        | 0.92          |
| (1,478) | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 12       | 0.92          |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD21 | 2        | 0.92          |
| (1,411) | 1:629:A:VAL:HG11 | 1:630:A:ALA:HB1  | 8        | 0.92          |
| (1,268) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HB3  | 18       | 0.92          |
| (1,268) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HB3  | 19       | 0.92          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 5        | 0.91          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 5        | 0.91          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 5        | 0.91          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 5        | 0.91          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 5        | 0.91          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 5        | 0.91          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 5        | 0.91          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 5        | 0.91          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 5        | 0.91          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 4        | 0.91          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 16       | 0.91          |
| (1,971) | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 5        | 0.91          |
| (1,857) | 1:636:A:GLU:H    | 1:635:A:VAL:HG21 | 4        | 0.91          |
| (1,857) | 1:636:A:GLU:H    | 1:635:A:VAL:HG22 | 17       | 0.91          |
| (1,787) | 1:616:A:ASP:H    | 1:614:A:THR:HG21 | 5        | 0.91          |
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD12 | 17       | 0.91          |
| (1,636) | 1:639:A:MET:HE2  | 1:639:A:MET:HA   | 17       | 0.91          |
| (1,613) | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 3        | 0.91          |
| (1,571) | 1:591:A:TRP:HD1  | 1:589:A:LYS:HA   | 19       | 0.91          |
| (1,478) | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 2        | 0.91          |
| (1,452) | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 4        | 0.91          |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD21 | 7        | 0.91          |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD22 | 14       | 0.91          |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD21 | 19       | 0.91          |
| (1,369) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD21 | 6        | 0.91          |
| (1,211) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD12 | 14       | 0.91          |
| (1,119) | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD12 | 6        | 0.91          |
| (1,119) | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD12 | 6        | 0.91          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 3        | 0.9           |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 3        | 0.9           |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 6        | 0.9           |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 6        | 0.9           |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 6        | 0.9           |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 6        | 0.9           |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 6        | 0.9           |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 6        | 0.9           |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 6        | 0.9           |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 6        | 0.9           |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 6        | 0.9           |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD11 | 7        | 0.9           |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD12 | 7        | 0.9           |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD13 | 7        | 0.9           |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD11 | 7        | 0.9           |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD12 | 7        | 0.9           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD13 | 7        | 0.9           |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 19       | 0.9           |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 19       | 0.9           |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 19       | 0.9           |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 19       | 0.9           |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 19       | 0.9           |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 19       | 0.9           |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 19       | 0.9           |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 19       | 0.9           |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 19       | 0.9           |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 2        | 0.9           |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 2        | 0.9           |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 2        | 0.9           |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 2        | 0.9           |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 2        | 0.9           |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 2        | 0.9           |
| (2,69)  | 2:534:B:PHE:HA   | 2:534:B:PHE:HD1  | 14       | 0.9           |
| (2,69)  | 2:534:B:PHE:HA   | 2:534:B:PHE:HD2  | 14       | 0.9           |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD23 | 16       | 0.9           |
| (1,971) | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 15       | 0.9           |
| (1,971) | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 17       | 0.9           |
| (1,971) | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 18       | 0.9           |
| (1,933) | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 2        | 0.9           |
| (1,933) | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 15       | 0.9           |
| (1,857) | 1:636:A:GLU:H    | 1:635:A:VAL:HG21 | 7        | 0.9           |
| (1,853) | 1:635:A:VAL:H    | 1:635:A:VAL:HG12 | 1        | 0.9           |
| (1,853) | 1:635:A:VAL:H    | 1:635:A:VAL:HG11 | 4        | 0.9           |
| (1,853) | 1:635:A:VAL:H    | 1:635:A:VAL:HG12 | 17       | 0.9           |
| (1,812) | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 15       | 0.9           |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 4        | 0.9           |
| (1,754) | 1:604:A:VAL:H    | 1:604:A:VAL:HG11 | 8        | 0.9           |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD13 | 12       | 0.9           |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 15       | 0.9           |
| (1,613) | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 4        | 0.9           |
| (1,613) | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 5        | 0.9           |
| (1,613) | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 9        | 0.9           |
| (1,600) | 1:646:A:ARG:HA   | 1:595:A:VAL:HG21 | 12       | 0.9           |
| (1,598) | 1:595:A:VAL:HG21 | 1:592:A:HIS:HA   | 1        | 0.9           |
| (1,596) | 1:632:A:ALA:HB3  | 1:635:A:VAL:HG22 | 18       | 0.9           |
| (1,593) | 1:634:A:LYS:HE2  | 1:634:A:LYS:HB2  | 5        | 0.9           |
| (1,535) | 1:639:A:MET:HG3  | 1:653:A:LEU:HD21 | 18       | 0.9           |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD22 | 7        | 0.9           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,478) | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 7        | 0.9           |
| (1,478) | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 8        | 0.9           |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD22 | 13       | 0.9           |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD21 | 16       | 0.9           |
| (1,260) | 1:587:A:VAL:HA   | 1:587:A:VAL:HG22 | 3        | 0.9           |
| (1,229) | 1:636:A:GLU:HG2  | 1:604:A:VAL:HG21 | 9        | 0.9           |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 14       | 0.9           |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 18       | 0.9           |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 18       | 0.9           |
| (1,141) | 1:595:A:VAL:HG23 | 1:640:A:TYR:HE1  | 4        | 0.9           |
| (1,141) | 1:595:A:VAL:HG23 | 1:640:A:TYR:HE2  | 4        | 0.9           |
| (1,98)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 3        | 0.9           |
| (2,95)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HB3  | 12       | 0.89          |
| (1,971) | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 9        | 0.89          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 7        | 0.89          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 8        | 0.89          |
| (1,933) | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 8        | 0.89          |
| (1,933) | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 9        | 0.89          |
| (1,933) | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 16       | 0.89          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 2        | 0.89          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 2        | 0.89          |
| (1,787) | 1:616:A:ASP:H    | 1:614:A:THR:HG21 | 17       | 0.89          |
| (1,654) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 13       | 0.89          |
| (1,639) | 1:652:A:LEU:HD23 | 1:642:A:SER:HB2  | 18       | 0.89          |
| (1,613) | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 6        | 0.89          |
| (1,613) | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 12       | 0.89          |
| (1,583) | 1:603:A:LEU:HD11 | 1:599:A:LEU:HD11 | 2        | 0.89          |
| (1,496) | 1:599:A:LEU:HD11 | 1:603:A:LEU:HD23 | 2        | 0.89          |
| (1,478) | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 4        | 0.89          |
| (1,478) | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 6        | 0.89          |
| (1,478) | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 14       | 0.89          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 4        | 0.89          |
| (1,452) | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 6        | 0.89          |
| (1,452) | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 20       | 0.89          |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD23 | 15       | 0.89          |
| (1,332) | 1:632:A:ALA:HB2  | 1:611:A:ILE:HD11 | 3        | 0.89          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 6        | 0.89          |
| (1,278) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 14       | 0.89          |
| (1,268) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HB3  | 16       | 0.89          |
| (1,207) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD12 | 17       | 0.89          |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 1        | 0.89          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 3        | 0.89          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 7        | 0.88          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 14       | 0.88          |
| (1,971)  | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 1        | 0.88          |
| (1,933)  | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 19       | 0.88          |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 15       | 0.88          |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 15       | 0.88          |
| (1,812)  | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 3        | 0.88          |
| (1,812)  | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 4        | 0.88          |
| (1,812)  | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 13       | 0.88          |
| (1,812)  | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 16       | 0.88          |
| (1,802)  | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 20       | 0.88          |
| (1,754)  | 1:604:A:VAL:H    | 1:604:A:VAL:HG13 | 5        | 0.88          |
| (1,715)  | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 10       | 0.88          |
| (1,654)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 3        | 0.88          |
| (1,613)  | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 2        | 0.88          |
| (1,613)  | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 10       | 0.88          |
| (1,613)  | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 14       | 0.88          |
| (1,610)  | 1:599:A:LEU:HD22 | 1:603:A:LEU:HD23 | 2        | 0.88          |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD1  | 15       | 0.88          |
| (1,597)  | 1:635:A:VAL:HG13 | 1:631:A:TYR:HD2  | 15       | 0.88          |
| (1,596)  | 1:632:A:ALA:HB1  | 1:635:A:VAL:HG21 | 10       | 0.88          |
| (1,536)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD21 | 9        | 0.88          |
| (1,485)  | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 2        | 0.88          |
| (1,484)  | 1:607:A:LEU:HD22 | 1:653:A:LEU:HB2  | 8        | 0.88          |
| (1,478)  | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 11       | 0.88          |
| (1,452)  | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 2        | 0.88          |
| (1,423)  | 1:629:A:VAL:HG13 | 1:626:A:GLU:HG2  | 20       | 0.88          |
| (1,13)   | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 13       | 0.88          |
| (1,971)  | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 8        | 0.87          |
| (1,933)  | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 18       | 0.87          |
| (1,875)  | 1:645:A:SER:H    | 1:648:A:GLU:HB2  | 10       | 0.87          |
| (1,857)  | 1:636:A:GLU:H    | 1:635:A:VAL:HG21 | 16       | 0.87          |
| (1,802)  | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 18       | 0.87          |
| (1,717)  | 1:610:A:ALA:H    | 1:657:A:ILE:HD13 | 18       | 0.87          |
| (1,654)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 4        | 0.87          |
| (1,654)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 16       | 0.87          |
| (1,641)  | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD12 | 1        | 0.87          |
| (1,621)  | 1:628:A:LEU:HD12 | 1:628:A:LEU:HA   | 6        | 0.87          |
| (1,613)  | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 16       | 0.87          |
| (1,548)  | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 13       | 0.87          |
| (1,509)  | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 16       | 0.87          |
| (1,478)  | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 16       | 0.87          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,464)  | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 11       | 0.87          |
| (1,374)  | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG11 | 14       | 0.87          |
| (1,364)  | 1:648:A:GLU:HA   | 1:651:A:HIS:HB2  | 19       | 0.87          |
| (1,345)  | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD12 | 15       | 0.87          |
| (1,332)  | 1:632:A:ALA:HB3  | 1:611:A:ILE:HD11 | 14       | 0.87          |
| (1,281)  | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 1        | 0.87          |
| (1,278)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 8        | 0.87          |
| (1,270)  | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 1        | 0.87          |
| (1,212)  | 1:611:A:ILE:HD11 | 1:607:A:LEU:HD21 | 11       | 0.87          |
| (1,212)  | 1:611:A:ILE:HD12 | 1:607:A:LEU:HD21 | 11       | 0.87          |
| (1,212)  | 1:611:A:ILE:HD13 | 1:607:A:LEU:HD21 | 11       | 0.87          |
| (1,194)  | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 18       | 0.87          |
| (1,163)  | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 19       | 0.87          |
| (1,13)   | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 8        | 0.87          |
| (2,276)  | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 10       | 0.86          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 3        | 0.86          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 3        | 0.86          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 3        | 0.86          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 5        | 0.86          |
| (1,986)  | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 2        | 0.86          |
| (1,971)  | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 2        | 0.86          |
| (1,939)  | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 1        | 0.86          |
| (1,933)  | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 5        | 0.86          |
| (1,933)  | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 13       | 0.86          |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 4        | 0.86          |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 4        | 0.86          |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 19       | 0.86          |
| (1,885)  | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 19       | 0.86          |
| (1,853)  | 1:635:A:VAL:H    | 1:635:A:VAL:HG12 | 7        | 0.86          |
| (1,853)  | 1:635:A:VAL:H    | 1:635:A:VAL:HG13 | 9        | 0.86          |
| (1,754)  | 1:604:A:VAL:H    | 1:604:A:VAL:HG13 | 1        | 0.86          |
| (1,725)  | 1:591:A:TRP:HE1  | 1:589:A:LYS:HG3  | 13       | 0.86          |
| (1,723)  | 1:609:A:GLN:H    | 1:608:A:VAL:HG11 | 17       | 0.86          |
| (1,613)  | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 8        | 0.86          |
| (1,613)  | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 18       | 0.86          |
| (1,613)  | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 19       | 0.86          |
| (1,452)  | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 8        | 0.86          |
| (1,452)  | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 10       | 0.86          |
| (1,452)  | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 19       | 0.86          |
| (1,411)  | 1:629:A:VAL:HG13 | 1:630:A:ALA:HB2  | 7        | 0.86          |
| (1,401)  | 1:616:A:ASP:HB2  | 1:619:A:ALA:HB2  | 18       | 0.86          |
| (1,394)  | 1:635:A:VAL:HG11 | 1:632:A:ALA:HA   | 12       | 0.86          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,194)  | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 10       | 0.86          |
| (1,30)   | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB1  | 20       | 0.86          |
| (1,13)   | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 19       | 0.86          |
| (3,4)    | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 7        | 0.85          |
| (3,4)    | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 7        | 0.85          |
| (3,4)    | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 7        | 0.85          |
| (3,4)    | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 7        | 0.85          |
| (3,4)    | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 7        | 0.85          |
| (3,4)    | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 7        | 0.85          |
| (2,168)  | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 19       | 0.85          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 18       | 0.85          |
| (1,983)  | 1:607:A:LEU:H    | 1:607:A:LEU:HD22 | 15       | 0.85          |
| (1,971)  | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 4        | 0.85          |
| (1,971)  | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 7        | 0.85          |
| (1,971)  | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 11       | 0.85          |
| (1,933)  | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 17       | 0.85          |
| (1,812)  | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 9        | 0.85          |
| (1,802)  | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 15       | 0.85          |
| (1,754)  | 1:604:A:VAL:H    | 1:604:A:VAL:HG11 | 10       | 0.85          |
| (1,715)  | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 8        | 0.85          |
| (1,601)  | 1:595:A:VAL:HG11 | 1:640:A:TYR:HD1  | 14       | 0.85          |
| (1,601)  | 1:595:A:VAL:HG11 | 1:640:A:TYR:HD2  | 14       | 0.85          |
| (1,485)  | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 8        | 0.85          |
| (1,479)  | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 5        | 0.85          |
| (1,464)  | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 19       | 0.85          |
| (1,461)  | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 20       | 0.85          |
| (1,452)  | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 18       | 0.85          |
| (1,332)  | 1:632:A:ALA:HB2  | 1:611:A:ILE:HD13 | 5        | 0.85          |
| (1,71)   | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 8        | 0.85          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 18       | 0.84          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 18       | 0.84          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 18       | 0.84          |
| (1,971)  | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 13       | 0.84          |
| (1,939)  | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 17       | 0.84          |
| (1,719)  | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 5        | 0.84          |
| (1,715)  | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 2        | 0.84          |
| (1,701)  | 1:614:A:THR:H    | 1:614:A:THR:HG21 | 12       | 0.84          |
| (1,654)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 2        | 0.84          |
| (1,654)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 15       | 0.84          |
| (1,624)  | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD12 | 5        | 0.84          |
| (1,624)  | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD12 | 5        | 0.84          |
| (1,610)  | 1:599:A:LEU:HD21 | 1:603:A:LEU:HD22 | 8        | 0.84          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,592) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HE2  | 4        | 0.84          |
| (1,332) | 1:632:A:ALA:HB1  | 1:611:A:ILE:HD11 | 1        | 0.84          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 15       | 0.84          |
| (1,167) | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 15       | 0.84          |
| (1,97)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HD3  | 3        | 0.84          |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB3  | 5        | 0.84          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 5        | 0.84          |
| (1,1)   | 1:656:A:LYS:HE2  | 1:639:A:MET:HE1  | 15       | 0.84          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 10       | 0.83          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 10       | 0.83          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 1        | 0.83          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 1        | 0.83          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 1        | 0.83          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 1        | 0.83          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 1        | 0.83          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 1        | 0.83          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 1        | 0.83          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 1        | 0.83          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 1        | 0.83          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 13       | 0.83          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 13       | 0.83          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 13       | 0.83          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 13       | 0.83          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 13       | 0.83          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 13       | 0.83          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 19       | 0.83          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 19       | 0.83          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 19       | 0.83          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 19       | 0.83          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 19       | 0.83          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 19       | 0.83          |
| (2,252) | 2:535:B:SER:H    | 2:534:B:PHE:HD1  | 3        | 0.83          |
| (2,169) | 2:544:B:ALA:HA   | 2:547:B:SER:HB3  | 2        | 0.83          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 13       | 0.83          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD11 | 7        | 0.83          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD12 | 7        | 0.83          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD13 | 7        | 0.83          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD11 | 7        | 0.83          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD12 | 7        | 0.83          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD13 | 7        | 0.83          |
| (1,992) | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 1        | 0.83          |
| (1,991) | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 1        | 0.83          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,754)  | 1:604:A:VAL:H    | 1:604:A:VAL:HG13 | 3        | 0.83          |
| (1,754)  | 1:604:A:VAL:H    | 1:604:A:VAL:HG13 | 4        | 0.83          |
| (1,754)  | 1:604:A:VAL:H    | 1:604:A:VAL:HG12 | 7        | 0.83          |
| (1,659)  | 1:652:A:LEU:HB3  | 1:639:A:MET:HE1  | 15       | 0.83          |
| (1,584)  | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD13 | 4        | 0.83          |
| (1,584)  | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD13 | 4        | 0.83          |
| (1,509)  | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 8        | 0.83          |
| (1,509)  | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 9        | 0.83          |
| (1,503)  | 1:625:A:MET:HG2  | 1:629:A:VAL:HG21 | 18       | 0.83          |
| (1,498)  | 1:639:A:MET:HG2  | 1:652:A:LEU:HD23 | 20       | 0.83          |
| (1,452)  | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 3        | 0.83          |
| (1,326)  | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 9        | 0.83          |
| (1,231)  | 1:601:A:SER:HA   | 1:604:A:VAL:HG21 | 19       | 0.83          |
| (1,999)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 6        | 0.82          |
| (1,999)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 6        | 0.82          |
| (1,999)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 6        | 0.82          |
| (1,998)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 6        | 0.82          |
| (1,998)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 6        | 0.82          |
| (1,998)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 6        | 0.82          |
| (1,983)  | 1:607:A:LEU:H    | 1:607:A:LEU:HD23 | 6        | 0.82          |
| (1,939)  | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 3        | 0.82          |
| (1,939)  | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 18       | 0.82          |
| (1,754)  | 1:604:A:VAL:H    | 1:604:A:VAL:HG11 | 14       | 0.82          |
| (1,754)  | 1:604:A:VAL:H    | 1:604:A:VAL:HG12 | 15       | 0.82          |
| (1,725)  | 1:591:A:TRP:HE1  | 1:589:A:LYS:HG3  | 6        | 0.82          |
| (1,723)  | 1:609:A:GLN:H    | 1:608:A:VAL:HG12 | 7        | 0.82          |
| (1,701)  | 1:614:A:THR:H    | 1:614:A:THR:HG23 | 7        | 0.82          |
| (1,658)  | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG23 | 2        | 0.82          |
| (1,644)  | 1:608:A:VAL:HA   | 1:611:A:ILE:HD13 | 19       | 0.82          |
| (1,639)  | 1:652:A:LEU:HD21 | 1:642:A:SER:HB2  | 12       | 0.82          |
| (1,610)  | 1:599:A:LEU:HD21 | 1:603:A:LEU:HD21 | 20       | 0.82          |
| (1,598)  | 1:595:A:VAL:HG21 | 1:592:A:HIS:HA   | 12       | 0.82          |
| (1,411)  | 1:629:A:VAL:HG13 | 1:630:A:ALA:HB2  | 10       | 0.82          |
| (1,354)  | 1:660:A:ILE:HD13 | 1:657:A:ILE:HA   | 7        | 0.82          |
| (1,354)  | 1:660:A:ILE:HD13 | 1:657:A:ILE:HA   | 13       | 0.82          |
| (1,227)  | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG23 | 11       | 0.82          |
| (1,227)  | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG21 | 13       | 0.82          |
| (1,227)  | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG22 | 18       | 0.82          |
| (1,219)  | 1:604:A:VAL:HA   | 1:607:A:LEU:HD21 | 14       | 0.82          |
| (1,87)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HE3  | 20       | 0.82          |
| (1,30)   | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB3  | 6        | 0.82          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 19       | 0.81          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,971) | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 16       | 0.81          |
| (1,857) | 1:636:A:GLU:H    | 1:635:A:VAL:HG21 | 6        | 0.81          |
| (1,853) | 1:635:A:VAL:H    | 1:635:A:VAL:HG11 | 20       | 0.81          |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 4        | 0.81          |
| (1,315) | 1:603:A:LEU:HA   | 1:603:A:LEU:HD12 | 12       | 0.81          |
| (1,278) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 5        | 0.81          |
| (1,219) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD22 | 12       | 0.81          |
| (1,857) | 1:636:A:GLU:H    | 1:635:A:VAL:HG22 | 3        | 0.8           |
| (1,857) | 1:636:A:GLU:H    | 1:635:A:VAL:HG21 | 8        | 0.8           |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 18       | 0.8           |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 17       | 0.8           |
| (1,754) | 1:604:A:VAL:H    | 1:604:A:VAL:HG12 | 16       | 0.8           |
| (1,721) | 1:609:A:GLN:H    | 1:608:A:VAL:HB   | 17       | 0.8           |
| (1,719) | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 1        | 0.8           |
| (1,719) | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 6        | 0.8           |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD11 | 6        | 0.8           |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 3        | 0.8           |
| (1,656) | 1:623:A:ARG:HG2  | 1:623:A:ARG:HA   | 20       | 0.8           |
| (1,654) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 11       | 0.8           |
| (1,636) | 1:639:A:MET:HE1  | 1:639:A:MET:HA   | 7        | 0.8           |
| (1,636) | 1:639:A:MET:HE2  | 1:639:A:MET:HA   | 12       | 0.8           |
| (1,598) | 1:595:A:VAL:HG21 | 1:592:A:HIS:HA   | 4        | 0.8           |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD23 | 8        | 0.8           |
| (1,475) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG13 | 3        | 0.8           |
| (1,354) | 1:660:A:ILE:HD11 | 1:657:A:ILE:HA   | 20       | 0.8           |
| (1,332) | 1:632:A:ALA:HB1  | 1:611:A:ILE:HD12 | 4        | 0.8           |
| (1,214) | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD13 | 7        | 0.8           |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 16       | 0.8           |
| (1,71)  | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 20       | 0.8           |
| (1,6)   | 1:608:A:VAL:HG13 | 1:625:A:MET:HE3  | 11       | 0.8           |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD21 | 20       | 0.79          |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD22 | 20       | 0.79          |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD23 | 20       | 0.79          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 4        | 0.79          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 16       | 0.79          |
| (2,95)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HB3  | 4        | 0.79          |
| (2,95)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HB3  | 11       | 0.79          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 11       | 0.79          |
| (1,857) | 1:636:A:GLU:H    | 1:635:A:VAL:HG22 | 11       | 0.79          |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 2        | 0.79          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 16       | 0.79          |
| (1,754) | 1:604:A:VAL:H    | 1:604:A:VAL:HG11 | 12       | 0.79          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,754) | 1:604:A:VAL:H    | 1:604:A:VAL:HG11 | 13       | 0.79          |
| (1,711) | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 1        | 0.79          |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 20       | 0.79          |
| (1,656) | 1:623:A:ARG:HG2  | 1:623:A:ARG:HA   | 5        | 0.79          |
| (1,656) | 1:623:A:ARG:HG2  | 1:623:A:ARG:HA   | 10       | 0.79          |
| (1,656) | 1:623:A:ARG:HG2  | 1:623:A:ARG:HA   | 18       | 0.79          |
| (1,592) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HE2  | 3        | 0.79          |
| (1,581) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 15       | 0.79          |
| (1,503) | 1:625:A:MET:HG2  | 1:629:A:VAL:HG22 | 1        | 0.79          |
| (1,475) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG12 | 6        | 0.79          |
| (1,452) | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 5        | 0.79          |
| (1,435) | 1:653:A:LEU:HD11 | 1:639:A:MET:HE1  | 4        | 0.79          |
| (1,411) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HB3  | 6        | 0.79          |
| (1,411) | 1:629:A:VAL:HG11 | 1:630:A:ALA:HB1  | 12       | 0.79          |
| (1,354) | 1:660:A:ILE:HD12 | 1:657:A:ILE:HA   | 17       | 0.79          |
| (1,354) | 1:660:A:ILE:HD12 | 1:657:A:ILE:HA   | 19       | 0.79          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 14       | 0.79          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 2        | 0.79          |
| (1,278) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 12       | 0.79          |
| (1,214) | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD11 | 3        | 0.79          |
| (1,212) | 1:611:A:ILE:HD11 | 1:607:A:LEU:HD22 | 9        | 0.79          |
| (1,212) | 1:611:A:ILE:HD12 | 1:607:A:LEU:HD22 | 9        | 0.79          |
| (1,212) | 1:611:A:ILE:HD13 | 1:607:A:LEU:HD22 | 9        | 0.79          |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 4        | 0.79          |
| (1,7)   | 1:628:A:LEU:HD23 | 1:625:A:MET:HE2  | 3        | 0.79          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 16       | 0.78          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 16       | 0.78          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD1  | 4        | 0.78          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD2  | 4        | 0.78          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD1  | 4        | 0.78          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD2  | 4        | 0.78          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD1  | 4        | 0.78          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD2  | 4        | 0.78          |
| (1,983) | 1:607:A:LEU:H    | 1:607:A:LEU:HD23 | 17       | 0.78          |
| (1,975) | 1:655:A:GLU:H    | 1:655:A:GLU:HB2  | 14       | 0.78          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 12       | 0.78          |
| (1,853) | 1:635:A:VAL:H    | 1:635:A:VAL:HG11 | 14       | 0.78          |
| (1,754) | 1:604:A:VAL:H    | 1:604:A:VAL:HG13 | 20       | 0.78          |
| (1,721) | 1:609:A:GLN:H    | 1:608:A:VAL:HB   | 1        | 0.78          |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG21 | 6        | 0.78          |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG21 | 11       | 0.78          |
| (1,636) | 1:639:A:MET:HE3  | 1:639:A:MET:HA   | 16       | 0.78          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,610)  | 1:599:A:LEU:HD23 | 1:603:A:LEU:HD22 | 7        | 0.78          |
| (1,452)  | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 15       | 0.78          |
| (1,441)  | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD23 | 11       | 0.78          |
| (1,364)  | 1:648:A:GLU:HA   | 1:651:A:HIS:HB2  | 18       | 0.78          |
| (1,332)  | 1:632:A:ALA:HB3  | 1:611:A:ILE:HD13 | 8        | 0.78          |
| (1,188)  | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 3        | 0.78          |
| (1,188)  | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 8        | 0.78          |
| (1,188)  | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 14       | 0.78          |
| (1,188)  | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 18       | 0.78          |
| (1,143)  | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 12       | 0.78          |
| (1,143)  | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 12       | 0.78          |
| (2,276)  | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 18       | 0.77          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG11 | 14       | 0.77          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG12 | 14       | 0.77          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG13 | 14       | 0.77          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG11 | 14       | 0.77          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG12 | 14       | 0.77          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG13 | 14       | 0.77          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG11 | 14       | 0.77          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG12 | 14       | 0.77          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG13 | 14       | 0.77          |
| (1,857)  | 1:636:A:GLU:H    | 1:635:A:VAL:HG21 | 2        | 0.77          |
| (1,812)  | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 6        | 0.77          |
| (1,812)  | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 19       | 0.77          |
| (1,754)  | 1:604:A:VAL:H    | 1:604:A:VAL:HG11 | 9        | 0.77          |
| (1,754)  | 1:604:A:VAL:H    | 1:604:A:VAL:HG11 | 17       | 0.77          |
| (1,719)  | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 4        | 0.77          |
| (1,699)  | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 6        | 0.77          |
| (1,699)  | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 7        | 0.77          |
| (1,659)  | 1:652:A:LEU:HB3  | 1:639:A:MET:HE2  | 5        | 0.77          |
| (1,613)  | 1:589:A:LYS:HD2  | 1:589:A:LYS:HA   | 1        | 0.77          |
| (1,484)  | 1:607:A:LEU:HD23 | 1:653:A:LEU:HB2  | 11       | 0.77          |
| (1,411)  | 1:629:A:VAL:HG12 | 1:630:A:ALA:HB2  | 9        | 0.77          |
| (1,411)  | 1:629:A:VAL:HG13 | 1:630:A:ALA:HB1  | 16       | 0.77          |
| (1,411)  | 1:629:A:VAL:HG12 | 1:630:A:ALA:HB3  | 20       | 0.77          |
| (1,374)  | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG13 | 16       | 0.77          |
| (1,366)  | 1:639:A:MET:HE3  | 1:653:A:LEU:HD23 | 8        | 0.77          |
| (1,332)  | 1:632:A:ALA:HB1  | 1:611:A:ILE:HD13 | 9        | 0.77          |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 9        | 0.77          |
| (1,281)  | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 9        | 0.77          |
| (1,271)  | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 2        | 0.77          |
| (1,271)  | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 10       | 0.77          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 11       | 0.77          |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 15       | 0.77          |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 20       | 0.77          |
| (1,268) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HB3  | 5        | 0.77          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 2        | 0.77          |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG21 | 4        | 0.77          |
| (1,214) | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD12 | 12       | 0.77          |
| (1,211) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD11 | 12       | 0.77          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 2        | 0.77          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 6        | 0.77          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 9        | 0.77          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 10       | 0.77          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 16       | 0.77          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 17       | 0.77          |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB3  | 11       | 0.77          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 4        | 0.76          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 4        | 0.76          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 4        | 0.76          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 4        | 0.76          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 4        | 0.76          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 4        | 0.76          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 4        | 0.76          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 4        | 0.76          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 4        | 0.76          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 18       | 0.76          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 18       | 0.76          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 18       | 0.76          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 18       | 0.76          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 18       | 0.76          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 18       | 0.76          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 18       | 0.76          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 18       | 0.76          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 18       | 0.76          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 2        | 0.76          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 2        | 0.76          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 2        | 0.76          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 2        | 0.76          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 2        | 0.76          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 2        | 0.76          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 19       | 0.76          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE1  | 12       | 0.76          |
| (1,885) | 1:650:A:TYR:H    | 1:649:A:TYR:HE2  | 12       | 0.76          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,719) | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 18       | 0.76          |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 11       | 0.76          |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 12       | 0.76          |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 14       | 0.76          |
| (1,598) | 1:595:A:VAL:HG21 | 1:592:A:HIS:HA   | 19       | 0.76          |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD11 | 2        | 0.76          |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD11 | 2        | 0.76          |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD13 | 11       | 0.76          |
| (1,411) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HB2  | 4        | 0.76          |
| (1,354) | 1:660:A:ILE:HD13 | 1:657:A:ILE:HA   | 3        | 0.76          |
| (1,302) | 1:614:A:THR:HG21 | 1:617:A:PRO:HA   | 2        | 0.76          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 5        | 0.76          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 17       | 0.76          |
| (1,278) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 18       | 0.76          |
| (1,219) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD21 | 3        | 0.76          |
| (1,209) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD22 | 8        | 0.76          |
| (1,209) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD23 | 20       | 0.76          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 1        | 0.76          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 13       | 0.76          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 15       | 0.76          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 20       | 0.76          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE1  | 12       | 0.75          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE2  | 12       | 0.75          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE1  | 12       | 0.75          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE2  | 12       | 0.75          |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE1  | 12       | 0.75          |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE2  | 12       | 0.75          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 20       | 0.75          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 20       | 0.75          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 5        | 0.75          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 5        | 0.75          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 5        | 0.75          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 5        | 0.75          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 5        | 0.75          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 5        | 0.75          |
| (2,252) | 2:535:B:SER:H    | 2:534:B:PHE:HD1  | 15       | 0.75          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD1  | 16       | 0.75          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD2  | 16       | 0.75          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD1  | 16       | 0.75          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD2  | 16       | 0.75          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD1  | 16       | 0.75          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD2  | 16       | 0.75          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,971) | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 3        | 0.75          |
| (1,939) | 1:664:A:LEU:H    | 1:663:A:GLU:HG2  | 15       | 0.75          |
| (1,875) | 1:645:A:SER:H    | 1:648:A:GLU:HB2  | 2        | 0.75          |
| (1,721) | 1:609:A:GLN:H    | 1:608:A:VAL:HB   | 7        | 0.75          |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD12 | 5        | 0.75          |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD11 | 13       | 0.75          |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 4        | 0.75          |
| (1,636) | 1:639:A:MET:HE1  | 1:639:A:MET:HA   | 10       | 0.75          |
| (1,598) | 1:595:A:VAL:HG22 | 1:592:A:HIS:HA   | 7        | 0.75          |
| (1,581) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 3        | 0.75          |
| (1,571) | 1:591:A:TRP:HD1  | 1:589:A:LYS:HA   | 17       | 0.75          |
| (1,523) | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD2  | 4        | 0.75          |
| (1,453) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HA   | 11       | 0.75          |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD22 | 17       | 0.75          |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD22 | 6        | 0.75          |
| (1,345) | 1:606:A:LYS:HB2  | 1:657:A:ILE:HD13 | 12       | 0.75          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 3        | 0.75          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 7        | 0.75          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 12       | 0.75          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 15       | 0.75          |
| (1,219) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD22 | 7        | 0.75          |
| (1,211) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD13 | 3        | 0.75          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 4        | 0.75          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 7        | 0.75          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 11       | 0.75          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 19       | 0.75          |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 20       | 0.75          |
| (1,117) | 1:653:A:LEU:HD22 | 1:650:A:TYR:HD1  | 7        | 0.75          |
| (1,117) | 1:653:A:LEU:HD22 | 1:650:A:TYR:HD2  | 7        | 0.75          |
| (1,97)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HD3  | 20       | 0.75          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 7        | 0.74          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 7        | 0.74          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 18       | 0.74          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 18       | 0.74          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 18       | 0.74          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 18       | 0.74          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 18       | 0.74          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 18       | 0.74          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 10       | 0.74          |
| (2,69)  | 2:534:B:PHE:HA   | 2:534:B:PHE:HD1  | 2        | 0.74          |
| (2,69)  | 2:534:B:PHE:HA   | 2:534:B:PHE:HD2  | 2        | 0.74          |
| (1,699) | 1:614:A:THR:H    | 1:615:A:PRO:HD2  | 2        | 0.74          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,656) | 1:623:A:ARG:HG2  | 1:623:A:ARG:HA   | 17       | 0.74          |
| (1,636) | 1:639:A:MET:HE2  | 1:639:A:MET:HA   | 4        | 0.74          |
| (1,606) | 1:595:A:VAL:HA   | 1:599:A:LEU:HD23 | 17       | 0.74          |
| (1,603) | 1:599:A:LEU:HD11 | 1:595:A:VAL:HG11 | 1        | 0.74          |
| (1,513) | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 15       | 0.74          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 3        | 0.74          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 6        | 0.74          |
| (1,452) | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 12       | 0.74          |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG13 | 7        | 0.74          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 13       | 0.74          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 20       | 0.74          |
| (1,278) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 17       | 0.74          |
| (1,207) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD13 | 11       | 0.74          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 1        | 0.73          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 1        | 0.73          |
| (2,250) | 2:534:B:PHE:H    | 2:534:B:PHE:HD1  | 6        | 0.73          |
| (2,95)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HB3  | 7        | 0.73          |
| (1,754) | 1:604:A:VAL:H    | 1:604:A:VAL:HG13 | 6        | 0.73          |
| (1,754) | 1:604:A:VAL:H    | 1:604:A:VAL:HG11 | 18       | 0.73          |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD12 | 7        | 0.73          |
| (1,606) | 1:595:A:VAL:HA   | 1:599:A:LEU:HD21 | 18       | 0.73          |
| (1,601) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HD1  | 5        | 0.73          |
| (1,601) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HD2  | 5        | 0.73          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 7        | 0.73          |
| (1,435) | 1:653:A:LEU:HD13 | 1:639:A:MET:HE2  | 10       | 0.73          |
| (1,332) | 1:632:A:ALA:HB1  | 1:611:A:ILE:HD12 | 6        | 0.73          |
| (1,278) | 1:623:A:ARG:HD2  | 1:623:A:ARG:HB2  | 20       | 0.73          |
| (1,214) | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD13 | 14       | 0.73          |
| (1,211) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD12 | 7        | 0.73          |
| (1,194) | 1:650:A:TYR:HB3  | 1:647:A:ASP:HA   | 7        | 0.73          |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB2  | 13       | 0.73          |
| (3,12)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD11 | 13       | 0.72          |
| (3,12)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD12 | 13       | 0.72          |
| (3,12)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD13 | 13       | 0.72          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 1        | 0.72          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 1        | 0.72          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 1        | 0.72          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 1        | 0.72          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 1        | 0.72          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 1        | 0.72          |
| (2,137) | 2:543:B:SER:HA   | 2:546:B:LEU:HB2  | 20       | 0.72          |
| (2,72)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HD1  | 16       | 0.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,72)   | 2:537:B:ILE:HB   | 2:534:B:PHE:HD2  | 16       | 0.72          |
| (1,754)  | 1:604:A:VAL:H    | 1:604:A:VAL:HG11 | 11       | 0.72          |
| (1,701)  | 1:614:A:THR:H    | 1:614:A:THR:HG21 | 2        | 0.72          |
| (1,658)  | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG23 | 3        | 0.72          |
| (1,610)  | 1:599:A:LEU:HD21 | 1:603:A:LEU:HD21 | 6        | 0.72          |
| (1,503)  | 1:625:A:MET:HG2  | 1:629:A:VAL:HG21 | 5        | 0.72          |
| (1,452)  | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 17       | 0.72          |
| (1,441)  | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD21 | 18       | 0.72          |
| (1,423)  | 1:629:A:VAL:HG13 | 1:626:A:GLU:HG2  | 18       | 0.72          |
| (1,367)  | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD22 | 9        | 0.72          |
| (1,359)  | 1:603:A:LEU:HD11 | 1:599:A:LEU:HD23 | 12       | 0.72          |
| (1,354)  | 1:660:A:ILE:HD11 | 1:657:A:ILE:HA   | 2        | 0.72          |
| (1,281)  | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 6        | 0.72          |
| (1,281)  | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 10       | 0.72          |
| (1,281)  | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 19       | 0.72          |
| (1,271)  | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 5        | 0.72          |
| (1,271)  | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 18       | 0.72          |
| (1,211)  | 1:604:A:VAL:HA   | 1:607:A:LEU:HD13 | 17       | 0.72          |
| (1,122)  | 1:595:A:VAL:HG21 | 1:649:A:TYR:HE1  | 12       | 0.72          |
| (1,122)  | 1:595:A:VAL:HG21 | 1:649:A:TYR:HE2  | 12       | 0.72          |
| (1,30)   | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB2  | 2        | 0.72          |
| (1,5)    | 1:608:A:VAL:HG21 | 1:625:A:MET:HE3  | 1        | 0.72          |
| (2,135)  | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 7        | 0.71          |
| (2,135)  | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 7        | 0.71          |
| (2,135)  | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 7        | 0.71          |
| (2,135)  | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 18       | 0.71          |
| (2,135)  | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 18       | 0.71          |
| (2,135)  | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 18       | 0.71          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 12       | 0.71          |
| (1,992)  | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 3        | 0.71          |
| (1,991)  | 1:643:A:ALA:HA   | 1:648:A:GLU:HG3  | 3        | 0.71          |
| (1,974)  | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 4        | 0.71          |
| (1,974)  | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 19       | 0.71          |
| (1,879)  | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 9        | 0.71          |
| (1,846)  | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 6        | 0.71          |
| (1,802)  | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 11       | 0.71          |
| (1,766)  | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 15       | 0.71          |
| (1,719)  | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 3        | 0.71          |
| (1,719)  | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 16       | 0.71          |
| (1,719)  | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 20       | 0.71          |
| (1,654)  | 1:623:A:ARG:HD2  | 1:623:A:ARG:HA   | 10       | 0.71          |
| (1,636)  | 1:639:A:MET:HE1  | 1:639:A:MET:HA   | 18       | 0.71          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,601) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HD1  | 18       | 0.71          |
| (1,601) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HD2  | 18       | 0.71          |
| (1,598) | 1:595:A:VAL:HG23 | 1:592:A:HIS:HA   | 15       | 0.71          |
| (1,540) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD13 | 9        | 0.71          |
| (1,513) | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 13       | 0.71          |
| (1,332) | 1:632:A:ALA:HB2  | 1:611:A:ILE:HD12 | 15       | 0.71          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 16       | 0.71          |
| (1,273) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HA   | 11       | 0.71          |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG23 | 7        | 0.71          |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG21 | 15       | 0.71          |
| (1,207) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD11 | 9        | 0.71          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB1  | 5        | 0.71          |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB1  | 3        | 0.71          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 10       | 0.7           |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 10       | 0.7           |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 10       | 0.7           |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 10       | 0.7           |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 10       | 0.7           |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 10       | 0.7           |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 10       | 0.7           |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 10       | 0.7           |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 10       | 0.7           |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 16       | 0.7           |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 16       | 0.7           |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 16       | 0.7           |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 16       | 0.7           |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 16       | 0.7           |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 16       | 0.7           |
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 3        | 0.7           |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 3        | 0.7           |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 3        | 0.7           |
| (2,95)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HB3  | 13       | 0.7           |
| (2,72)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HD1  | 12       | 0.7           |
| (2,72)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HD2  | 12       | 0.7           |
| (1,974) | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 1        | 0.7           |
| (1,974) | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 10       | 0.7           |
| (1,974) | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 18       | 0.7           |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 12       | 0.7           |
| (1,875) | 1:645:A:SER:H    | 1:648:A:GLU:HB2  | 4        | 0.7           |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 13       | 0.7           |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG21 | 1        | 0.7           |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG22 | 5        | 0.7           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,812) | 1:624:A:ARG:H    | 1:623:A:ARG:HG2  | 2        | 0.7           |
| (1,725) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HG3  | 5        | 0.7           |
| (1,719) | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 9        | 0.7           |
| (1,641) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD13 | 15       | 0.7           |
| (1,620) | 1:625:A:MET:HG2  | 1:620:A:LEU:HD12 | 7        | 0.7           |
| (1,589) | 1:599:A:LEU:HD23 | 1:599:A:LEU:HB2  | 1        | 0.7           |
| (1,589) | 1:599:A:LEU:HD23 | 1:599:A:LEU:HB2  | 14       | 0.7           |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 4        | 0.7           |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD12 | 6        | 0.7           |
| (1,417) | 1:656:A:LYS:HB2  | 1:660:A:ILE:HD13 | 12       | 0.7           |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG12 | 20       | 0.7           |
| (1,364) | 1:648:A:GLU:HA   | 1:651:A:HIS:HB2  | 3        | 0.7           |
| (1,332) | 1:632:A:ALA:HB1  | 1:611:A:ILE:HD13 | 11       | 0.7           |
| (1,290) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 7        | 0.7           |
| (1,290) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 9        | 0.7           |
| (1,290) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 11       | 0.7           |
| (1,290) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 13       | 0.7           |
| (1,290) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 16       | 0.7           |
| (1,209) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD23 | 15       | 0.7           |
| (1,209) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD21 | 16       | 0.7           |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 9        | 0.7           |
| (1,118) | 1:653:A:LEU:HB3  | 1:650:A:TYR:HA   | 10       | 0.7           |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB2  | 4        | 0.7           |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB2  | 7        | 0.7           |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB3  | 10       | 0.7           |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB3  | 17       | 0.7           |
| (1,7)   | 1:628:A:LEU:HD22 | 1:625:A:MET:HE2  | 7        | 0.7           |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 11       | 0.69          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 11       | 0.69          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 11       | 0.69          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 11       | 0.69          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 11       | 0.69          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 11       | 0.69          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 11       | 0.69          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 11       | 0.69          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 11       | 0.69          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 16       | 0.69          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 16       | 0.69          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 17       | 0.69          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 17       | 0.69          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 17       | 0.69          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 17       | 0.69          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 17       | 0.69          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 17       | 0.69          |
| (2,252) | 2:535:B:SER:H    | 2:534:B:PHE:HD1  | 13       | 0.69          |
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 17       | 0.69          |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 17       | 0.69          |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 17       | 0.69          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD1  | 6        | 0.69          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD2  | 6        | 0.69          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD1  | 6        | 0.69          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD2  | 6        | 0.69          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD1  | 6        | 0.69          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD2  | 6        | 0.69          |
| (1,974) | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 15       | 0.69          |
| (1,933) | 1:662:A:LYS:H    | 1:662:A:LYS:HG2  | 14       | 0.69          |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 7        | 0.69          |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 10       | 0.69          |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 10       | 0.69          |
| (1,754) | 1:604:A:VAL:H    | 1:604:A:VAL:HG11 | 2        | 0.69          |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD12 | 16       | 0.69          |
| (1,701) | 1:614:A:THR:H    | 1:614:A:THR:HG22 | 1        | 0.69          |
| (1,636) | 1:639:A:MET:HE2  | 1:639:A:MET:HA   | 1        | 0.69          |
| (1,572) | 1:654:A:ALA:HB2  | 1:657:A:ILE:HD12 | 3        | 0.69          |
| (1,548) | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 14       | 0.69          |
| (1,548) | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 16       | 0.69          |
| (1,469) | 1:635:A:VAL:HA   | 1:635:A:VAL:HG13 | 13       | 0.69          |
| (1,464) | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 13       | 0.69          |
| (1,384) | 1:614:A:THR:HG21 | 1:614:A:THR:HA   | 20       | 0.69          |
| (1,326) | 1:663:A:GLU:HB3  | 1:660:A:ILE:HA   | 18       | 0.69          |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 16       | 0.69          |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 19       | 0.69          |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG22 | 3        | 0.69          |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG23 | 16       | 0.69          |
| (1,212) | 1:611:A:ILE:HD11 | 1:607:A:LEU:HD23 | 2        | 0.69          |
| (1,212) | 1:611:A:ILE:HD12 | 1:607:A:LEU:HD23 | 2        | 0.69          |
| (1,212) | 1:611:A:ILE:HD13 | 1:607:A:LEU:HD23 | 2        | 0.69          |
| (1,212) | 1:611:A:ILE:HD11 | 1:607:A:LEU:HD21 | 20       | 0.69          |
| (1,212) | 1:611:A:ILE:HD12 | 1:607:A:LEU:HD21 | 20       | 0.69          |
| (1,212) | 1:611:A:ILE:HD13 | 1:607:A:LEU:HD21 | 20       | 0.69          |
| (1,211) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD12 | 9        | 0.69          |
| (1,210) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD22 | 4        | 0.69          |
| (1,97)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HD3  | 12       | 0.69          |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB2  | 14       | 0.69          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB3  | 15       | 0.69          |
| (3,32)  | 1:664:A:LEU:HD11 | 2:542:B:PHE:HE1  | 7        | 0.68          |
| (3,32)  | 1:664:A:LEU:HD11 | 2:542:B:PHE:HE2  | 7        | 0.68          |
| (3,32)  | 1:664:A:LEU:HD12 | 2:542:B:PHE:HE1  | 7        | 0.68          |
| (3,32)  | 1:664:A:LEU:HD12 | 2:542:B:PHE:HE2  | 7        | 0.68          |
| (3,32)  | 1:664:A:LEU:HD13 | 2:542:B:PHE:HE1  | 7        | 0.68          |
| (3,32)  | 1:664:A:LEU:HD13 | 2:542:B:PHE:HE2  | 7        | 0.68          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 12       | 0.68          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 12       | 0.68          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 7        | 0.68          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 7        | 0.68          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 7        | 0.68          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 7        | 0.68          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 7        | 0.68          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 7        | 0.68          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 13       | 0.68          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 13       | 0.68          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 13       | 0.68          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 13       | 0.68          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 13       | 0.68          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 13       | 0.68          |
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 11       | 0.68          |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 11       | 0.68          |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 11       | 0.68          |
| (1,875) | 1:645:A:SER:H    | 1:648:A:GLU:HB2  | 16       | 0.68          |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 11       | 0.68          |
| (1,787) | 1:616:A:ASP:H    | 1:614:A:THR:HG21 | 3        | 0.68          |
| (1,745) | 1:600:A:ARG:H    | 1:599:A:LEU:HB2  | 11       | 0.68          |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB1  | 11       | 0.68          |
| (1,701) | 1:614:A:THR:H    | 1:614:A:THR:HG22 | 10       | 0.68          |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD22 | 10       | 0.68          |
| (1,598) | 1:595:A:VAL:HG21 | 1:592:A:HIS:HA   | 17       | 0.68          |
| (1,589) | 1:599:A:LEU:HD22 | 1:599:A:LEU:HB2  | 9        | 0.68          |
| (1,589) | 1:599:A:LEU:HD21 | 1:599:A:LEU:HB2  | 10       | 0.68          |
| (1,470) | 1:635:A:VAL:HG12 | 1:639:A:MET:HE3  | 17       | 0.68          |
| (1,457) | 1:608:A:VAL:HG23 | 1:605:A:HIS:HA   | 16       | 0.68          |
| (1,453) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HA   | 13       | 0.68          |
| (1,441) | 1:603:A:LEU:HB2  | 1:603:A:LEU:HD23 | 12       | 0.68          |
| (1,384) | 1:614:A:THR:HG23 | 1:614:A:THR:HA   | 4        | 0.68          |
| (1,290) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 1        | 0.68          |
| (1,290) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 3        | 0.68          |
| (1,290) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 4        | 0.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,290)  | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 10       | 0.68          |
| (1,290)  | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 12       | 0.68          |
| (1,290)  | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 15       | 0.68          |
| (1,290)  | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 17       | 0.68          |
| (1,290)  | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 20       | 0.68          |
| (1,281)  | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 14       | 0.68          |
| (1,125)  | 1:603:A:LEU:HD23 | 1:650:A:TYR:HE1  | 17       | 0.68          |
| (1,125)  | 1:603:A:LEU:HD23 | 1:650:A:TYR:HE2  | 17       | 0.68          |
| (1,119)  | 1:650:A:TYR:HE1  | 1:653:A:LEU:HD11 | 9        | 0.68          |
| (1,119)  | 1:650:A:TYR:HE2  | 1:653:A:LEU:HD11 | 9        | 0.68          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE1  | 14       | 0.68          |
| (1,109)  | 1:662:A:LYS:HD3  | 1:658:A:TYR:HE2  | 14       | 0.68          |
| (1,30)   | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB3  | 9        | 0.68          |
| (3,24)   | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 9        | 0.67          |
| (3,24)   | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 9        | 0.67          |
| (3,24)   | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 9        | 0.67          |
| (3,24)   | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 9        | 0.67          |
| (3,24)   | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 9        | 0.67          |
| (3,24)   | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 9        | 0.67          |
| (3,24)   | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 9        | 0.67          |
| (3,24)   | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 9        | 0.67          |
| (3,24)   | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 9        | 0.67          |
| (2,219)  | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 8        | 0.67          |
| (2,169)  | 2:544:B:ALA:HA   | 2:547:B:SER:HB3  | 3        | 0.67          |
| (2,135)  | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 6        | 0.67          |
| (2,135)  | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 6        | 0.67          |
| (2,135)  | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 6        | 0.67          |
| (2,135)  | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 10       | 0.67          |
| (2,135)  | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 10       | 0.67          |
| (2,135)  | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 10       | 0.67          |
| (2,135)  | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 16       | 0.67          |
| (2,135)  | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 16       | 0.67          |
| (2,135)  | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 16       | 0.67          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 3        | 0.67          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG11 | 3        | 0.67          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG12 | 3        | 0.67          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG13 | 3        | 0.67          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG11 | 3        | 0.67          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG12 | 3        | 0.67          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG13 | 3        | 0.67          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG11 | 3        | 0.67          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG12 | 3        | 0.67          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG13 | 3        | 0.67          |
| (1,993)  | 1:619:A:ALA:HB1  | 1:612:A:PHE:HZ   | 2        | 0.67          |
| (1,993)  | 1:619:A:ALA:HB2  | 1:612:A:PHE:HZ   | 2        | 0.67          |
| (1,993)  | 1:619:A:ALA:HB3  | 1:612:A:PHE:HZ   | 2        | 0.67          |
| (1,951)  | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 12       | 0.67          |
| (1,846)  | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 14       | 0.67          |
| (1,819)  | 1:598:A:ASP:H    | 1:596:A:THR:HG23 | 20       | 0.67          |
| (1,719)  | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 19       | 0.67          |
| (1,715)  | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 13       | 0.67          |
| (1,711)  | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 12       | 0.67          |
| (1,644)  | 1:608:A:VAL:HA   | 1:611:A:ILE:HD12 | 17       | 0.67          |
| (1,644)  | 1:608:A:VAL:HA   | 1:611:A:ILE:HD11 | 18       | 0.67          |
| (1,642)  | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD12 | 10       | 0.67          |
| (1,598)  | 1:595:A:VAL:HG22 | 1:592:A:HIS:HA   | 3        | 0.67          |
| (1,589)  | 1:599:A:LEU:HD22 | 1:599:A:LEU:HB2  | 5        | 0.67          |
| (1,589)  | 1:599:A:LEU:HD22 | 1:599:A:LEU:HB2  | 16       | 0.67          |
| (1,584)  | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD11 | 14       | 0.67          |
| (1,584)  | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD11 | 14       | 0.67          |
| (1,523)  | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD2  | 16       | 0.67          |
| (1,470)  | 1:635:A:VAL:HG11 | 1:639:A:MET:HE2  | 8        | 0.67          |
| (1,465)  | 1:589:A:LYS:HG2  | 1:589:A:LYS:HE2  | 19       | 0.67          |
| (1,411)  | 1:629:A:VAL:HG13 | 1:630:A:ALA:HB1  | 11       | 0.67          |
| (1,396)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HB2  | 4        | 0.67          |
| (1,396)  | 1:664:A:LEU:HD23 | 1:664:A:LEU:HB2  | 5        | 0.67          |
| (1,396)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HB2  | 14       | 0.67          |
| (1,396)  | 1:664:A:LEU:HD23 | 1:664:A:LEU:HB2  | 15       | 0.67          |
| (1,354)  | 1:660:A:ILE:HD11 | 1:657:A:ILE:HA   | 1        | 0.67          |
| (1,332)  | 1:632:A:ALA:HB2  | 1:611:A:ILE:HD13 | 7        | 0.67          |
| (1,332)  | 1:632:A:ALA:HB3  | 1:611:A:ILE:HD11 | 20       | 0.67          |
| (1,290)  | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 5        | 0.67          |
| (1,290)  | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 18       | 0.67          |
| (1,290)  | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 19       | 0.67          |
| (1,286)  | 1:671:A:ARG:HD2  | 1:671:A:ARG:HA   | 6        | 0.67          |
| (1,214)  | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD11 | 17       | 0.67          |
| (1,209)  | 1:607:A:LEU:HA   | 1:607:A:LEU:HD22 | 2        | 0.67          |
| (1,193)  | 1:650:A:TYR:HB2  | 1:647:A:ASP:HA   | 12       | 0.67          |
| (1,98)   | 1:662:A:LYS:HA   | 1:662:A:LYS:HD3  | 12       | 0.67          |
| (1,30)   | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB2  | 1        | 0.67          |
| (1,30)   | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB3  | 16       | 0.67          |
| (1,30)   | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB2  | 19       | 0.67          |
| (1,3)    | 1:639:A:MET:HG3  | 1:639:A:MET:HE2  | 1        | 0.67          |
| (2,219)  | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 5        | 0.66          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,219) | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 14       | 0.66          |
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 15       | 0.66          |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 15       | 0.66          |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 15       | 0.66          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD1  | 13       | 0.66          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD2  | 13       | 0.66          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD1  | 13       | 0.66          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD2  | 13       | 0.66          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD1  | 13       | 0.66          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD2  | 13       | 0.66          |
| (1,986) | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 13       | 0.66          |
| (1,974) | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 3        | 0.66          |
| (1,974) | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 5        | 0.66          |
| (1,935) | 1:663:A:GLU:H    | 1:663:A:GLU:HG2  | 4        | 0.66          |
| (1,932) | 1:662:A:LYS:H    | 1:662:A:LYS:HB3  | 20       | 0.66          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 8        | 0.66          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 11       | 0.66          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG21 | 7        | 0.66          |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 14       | 0.66          |
| (1,598) | 1:595:A:VAL:HG22 | 1:592:A:HIS:HA   | 10       | 0.66          |
| (1,596) | 1:632:A:ALA:HB1  | 1:635:A:VAL:HG22 | 19       | 0.66          |
| (1,589) | 1:599:A:LEU:HD23 | 1:599:A:LEU:HB2  | 13       | 0.66          |
| (1,572) | 1:654:A:ALA:HB1  | 1:657:A:ILE:HD12 | 2        | 0.66          |
| (1,571) | 1:591:A:TRP:HD1  | 1:589:A:LYS:HA   | 8        | 0.66          |
| (1,513) | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 11       | 0.66          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 20       | 0.66          |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD21 | 15       | 0.66          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 20       | 0.66          |
| (1,452) | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 14       | 0.66          |
| (1,411) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HB3  | 13       | 0.66          |
| (1,396) | 1:664:A:LEU:HD23 | 1:664:A:LEU:HB2  | 7        | 0.66          |
| (1,396) | 1:664:A:LEU:HD21 | 1:664:A:LEU:HB2  | 12       | 0.66          |
| (1,396) | 1:664:A:LEU:HD23 | 1:664:A:LEU:HB2  | 17       | 0.66          |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG13 | 13       | 0.66          |
| (1,366) | 1:639:A:MET:HE2  | 1:653:A:LEU:HD21 | 15       | 0.66          |
| (1,354) | 1:660:A:ILE:HD12 | 1:657:A:ILE:HA   | 9        | 0.66          |
| (1,354) | 1:660:A:ILE:HD13 | 1:657:A:ILE:HA   | 15       | 0.66          |
| (1,332) | 1:632:A:ALA:HB1  | 1:611:A:ILE:HD12 | 2        | 0.66          |
| (1,302) | 1:614:A:THR:HG21 | 1:617:A:PRO:HA   | 18       | 0.66          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 18       | 0.66          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG23 | 5        | 0.66          |
| (1,225) | 1:632:A:ALA:HB1  | 1:604:A:VAL:HG22 | 10       | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,211)  | 1:604:A:VAL:HA   | 1:607:A:LEU:HD12 | 16       | 0.66          |
| (1,209)  | 1:607:A:LEU:HA   | 1:607:A:LEU:HD23 | 11       | 0.66          |
| (1,93)   | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE2  | 2        | 0.66          |
| (1,93)   | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE2  | 10       | 0.66          |
| (1,93)   | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE2  | 18       | 0.66          |
| (1,93)   | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE2  | 19       | 0.66          |
| (3,24)   | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 13       | 0.65          |
| (3,24)   | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 13       | 0.65          |
| (3,24)   | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 13       | 0.65          |
| (3,24)   | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 13       | 0.65          |
| (3,24)   | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 13       | 0.65          |
| (3,24)   | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 13       | 0.65          |
| (3,24)   | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 13       | 0.65          |
| (3,24)   | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 13       | 0.65          |
| (3,24)   | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 13       | 0.65          |
| (3,19)   | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 1        | 0.65          |
| (3,19)   | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 1        | 0.65          |
| (3,19)   | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 1        | 0.65          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 1        | 0.65          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 1        | 0.65          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 1        | 0.65          |
| (2,169)  | 2:544:B:ALA:HA   | 2:547:B:SER:HB3  | 15       | 0.65          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 1        | 0.65          |
| (1,986)  | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 1        | 0.65          |
| (1,974)  | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 7        | 0.65          |
| (1,974)  | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 16       | 0.65          |
| (1,974)  | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 20       | 0.65          |
| (1,819)  | 1:598:A:ASP:H    | 1:596:A:THR:HG21 | 4        | 0.65          |
| (1,819)  | 1:598:A:ASP:H    | 1:596:A:THR:HG22 | 10       | 0.65          |
| (1,819)  | 1:598:A:ASP:H    | 1:596:A:THR:HG22 | 13       | 0.65          |
| (1,819)  | 1:598:A:ASP:H    | 1:596:A:THR:HG23 | 17       | 0.65          |
| (1,802)  | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 13       | 0.65          |
| (1,762)  | 1:605:A:HIS:H    | 1:604:A:VAL:HG22 | 19       | 0.65          |
| (1,745)  | 1:600:A:ARG:H    | 1:599:A:LEU:HB2  | 15       | 0.65          |
| (1,717)  | 1:610:A:ALA:H    | 1:657:A:ILE:HD11 | 10       | 0.65          |
| (1,711)  | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 2        | 0.65          |
| (1,657)  | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE1  | 19       | 0.65          |
| (1,657)  | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE2  | 19       | 0.65          |
| (1,636)  | 1:639:A:MET:HE3  | 1:639:A:MET:HA   | 2        | 0.65          |
| (1,580)  | 1:599:A:LEU:HD13 | 1:599:A:LEU:HA   | 1        | 0.65          |
| (1,503)  | 1:625:A:MET:HG2  | 1:629:A:VAL:HG23 | 19       | 0.65          |
| (1,498)  | 1:639:A:MET:HG2  | 1:652:A:LEU:HD21 | 4        | 0.65          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,475) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG13 | 15       | 0.65          |
| (1,470) | 1:635:A:VAL:HG13 | 1:639:A:MET:HE3  | 10       | 0.65          |
| (1,411) | 1:629:A:VAL:HG12 | 1:630:A:ALA:HB1  | 17       | 0.65          |
| (1,396) | 1:664:A:LEU:HD23 | 1:664:A:LEU:HB2  | 1        | 0.65          |
| (1,396) | 1:664:A:LEU:HD23 | 1:664:A:LEU:HB2  | 6        | 0.65          |
| (1,384) | 1:614:A:THR:HG22 | 1:614:A:THR:HA   | 14       | 0.65          |
| (1,354) | 1:660:A:ILE:HD13 | 1:657:A:ILE:HA   | 4        | 0.65          |
| (1,354) | 1:660:A:ILE:HD12 | 1:657:A:ILE:HA   | 8        | 0.65          |
| (1,332) | 1:632:A:ALA:HB3  | 1:611:A:ILE:HD12 | 17       | 0.65          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG22 | 2        | 0.65          |
| (1,207) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD11 | 8        | 0.65          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB2  | 13       | 0.65          |
| (1,172) | 1:651:A:HIS:HB2  | 1:651:A:HIS:HD2  | 12       | 0.65          |
| (1,172) | 1:651:A:HIS:HB2  | 1:651:A:HIS:HD2  | 13       | 0.65          |
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 8        | 0.64          |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 8        | 0.64          |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 8        | 0.64          |
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 19       | 0.64          |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 19       | 0.64          |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 19       | 0.64          |
| (1,974) | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 6        | 0.64          |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 16       | 0.64          |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG21 | 2        | 0.64          |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG23 | 8        | 0.64          |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG21 | 9        | 0.64          |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG21 | 11       | 0.64          |
| (1,802) | 1:621:A:LYS:H    | 1:622:A:ASP:HB3  | 6        | 0.64          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 3        | 0.64          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 7        | 0.64          |
| (1,745) | 1:600:A:ARG:H    | 1:599:A:LEU:HB2  | 19       | 0.64          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG23 | 19       | 0.64          |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB1  | 17       | 0.64          |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD12 | 15       | 0.64          |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD11 | 10       | 0.64          |
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD11 | 4        | 0.64          |
| (1,639) | 1:652:A:LEU:HD22 | 1:642:A:SER:HB2  | 5        | 0.64          |
| (1,598) | 1:595:A:VAL:HG23 | 1:592:A:HIS:HA   | 8        | 0.64          |
| (1,580) | 1:599:A:LEU:HD11 | 1:599:A:LEU:HA   | 9        | 0.64          |
| (1,548) | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 1        | 0.64          |
| (1,548) | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 3        | 0.64          |
| (1,524) | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD3  | 4        | 0.64          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 2        | 0.64          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 7        | 0.64          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 12       | 0.64          |
| (1,475) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG11 | 11       | 0.64          |
| (1,452) | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 13       | 0.64          |
| (1,396) | 1:664:A:LEU:HD23 | 1:664:A:LEU:HB2  | 9        | 0.64          |
| (1,384) | 1:614:A:THR:HG22 | 1:614:A:THR:HA   | 11       | 0.64          |
| (1,368) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD22 | 10       | 0.64          |
| (1,364) | 1:648:A:GLU:HA   | 1:651:A:HIS:HB2  | 2        | 0.64          |
| (1,354) | 1:660:A:ILE:HD12 | 1:657:A:ILE:HA   | 16       | 0.64          |
| (1,332) | 1:632:A:ALA:HB2  | 1:611:A:ILE:HD13 | 13       | 0.64          |
| (1,332) | 1:632:A:ALA:HB3  | 1:611:A:ILE:HD13 | 19       | 0.64          |
| (1,212) | 1:611:A:ILE:HD11 | 1:607:A:LEU:HD23 | 8        | 0.64          |
| (1,212) | 1:611:A:ILE:HD12 | 1:607:A:LEU:HD23 | 8        | 0.64          |
| (1,212) | 1:611:A:ILE:HD13 | 1:607:A:LEU:HD23 | 8        | 0.64          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE1  | 6        | 0.64          |
| (1,121) | 1:653:A:LEU:HD13 | 1:649:A:TYR:HE2  | 6        | 0.64          |
| (1,117) | 1:653:A:LEU:HD21 | 1:650:A:TYR:HD1  | 11       | 0.64          |
| (1,117) | 1:653:A:LEU:HD21 | 1:650:A:TYR:HD2  | 11       | 0.64          |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 2        | 0.64          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 15       | 0.64          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 8        | 0.63          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 8        | 0.63          |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD21 | 12       | 0.63          |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD22 | 12       | 0.63          |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD23 | 12       | 0.63          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD11 | 13       | 0.63          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD12 | 13       | 0.63          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD13 | 13       | 0.63          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD11 | 13       | 0.63          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD12 | 13       | 0.63          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD13 | 13       | 0.63          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG21 | 11       | 0.63          |
| (2,219) | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 2        | 0.63          |
| (2,219) | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 11       | 0.63          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 18       | 0.63          |
| (2,168) | 2:544:B:ALA:HA   | 2:547:B:SER:HB2  | 12       | 0.63          |
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 2        | 0.63          |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 2        | 0.63          |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 2        | 0.63          |
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 5        | 0.63          |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 5        | 0.63          |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 5        | 0.63          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 4        | 0.63          |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 5        | 0.63          |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 9        | 0.63          |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG21 | 6        | 0.63          |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG23 | 7        | 0.63          |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG23 | 12       | 0.63          |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 13       | 0.63          |
| (1,754) | 1:604:A:VAL:H    | 1:604:A:VAL:HG11 | 19       | 0.63          |
| (1,745) | 1:600:A:ARG:H    | 1:599:A:LEU:HB2  | 6        | 0.63          |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD11 | 4        | 0.63          |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG22 | 18       | 0.63          |
| (1,610) | 1:599:A:LEU:HD21 | 1:603:A:LEU:HD22 | 18       | 0.63          |
| (1,598) | 1:595:A:VAL:HG23 | 1:592:A:HIS:HA   | 5        | 0.63          |
| (1,598) | 1:595:A:VAL:HG22 | 1:592:A:HIS:HA   | 16       | 0.63          |
| (1,598) | 1:595:A:VAL:HG22 | 1:592:A:HIS:HA   | 20       | 0.63          |
| (1,583) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD11 | 5        | 0.63          |
| (1,580) | 1:599:A:LEU:HD13 | 1:599:A:LEU:HA   | 17       | 0.63          |
| (1,535) | 1:639:A:MET:HG3  | 1:653:A:LEU:HD21 | 12       | 0.63          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 1        | 0.63          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 3        | 0.63          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 5        | 0.63          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 9        | 0.63          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 10       | 0.63          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 17       | 0.63          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 18       | 0.63          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 11       | 0.63          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 14       | 0.63          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD21 | 16       | 0.63          |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD22 | 1        | 0.63          |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD23 | 16       | 0.63          |
| (1,495) | 1:653:A:LEU:HD13 | 1:603:A:LEU:HD13 | 20       | 0.63          |
| (1,457) | 1:608:A:VAL:HG23 | 1:605:A:HIS:HA   | 19       | 0.63          |
| (1,396) | 1:664:A:LEU:HD21 | 1:664:A:LEU:HB2  | 8        | 0.63          |
| (1,396) | 1:664:A:LEU:HD21 | 1:664:A:LEU:HB2  | 18       | 0.63          |
| (1,396) | 1:664:A:LEU:HD21 | 1:664:A:LEU:HB2  | 19       | 0.63          |
| (1,384) | 1:614:A:THR:HG22 | 1:614:A:THR:HA   | 6        | 0.63          |
| (1,332) | 1:632:A:ALA:HB2  | 1:611:A:ILE:HD11 | 18       | 0.63          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG23 | 9        | 0.63          |
| (1,229) | 1:636:A:GLU:HG2  | 1:604:A:VAL:HG23 | 5        | 0.63          |
| (1,211) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD11 | 11       | 0.63          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB1  | 14       | 0.63          |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 17       | 0.63          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 12       | 0.63          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 17       | 0.62          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 17       | 0.62          |
| (2,219) | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 20       | 0.62          |
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 9        | 0.62          |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 9        | 0.62          |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 9        | 0.62          |
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 14       | 0.62          |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 14       | 0.62          |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 14       | 0.62          |
| (2,133) | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 3        | 0.62          |
| (1,993) | 1:619:A:ALA:HB1  | 1:612:A:PHE:HZ   | 8        | 0.62          |
| (1,993) | 1:619:A:ALA:HB2  | 1:612:A:PHE:HZ   | 8        | 0.62          |
| (1,993) | 1:619:A:ALA:HB3  | 1:612:A:PHE:HZ   | 8        | 0.62          |
| (1,986) | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 8        | 0.62          |
| (1,974) | 1:655:A:GLU:H    | 1:655:A:GLU:HG3  | 2        | 0.62          |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 14       | 0.62          |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 17       | 0.62          |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 8        | 0.62          |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 2        | 0.62          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 2        | 0.62          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 12       | 0.62          |
| (1,701) | 1:614:A:THR:H    | 1:614:A:THR:HG22 | 15       | 0.62          |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD13 | 12       | 0.62          |
| (1,598) | 1:595:A:VAL:HG21 | 1:592:A:HIS:HA   | 18       | 0.62          |
| (1,580) | 1:599:A:LEU:HD11 | 1:599:A:LEU:HA   | 18       | 0.62          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 4        | 0.62          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 6        | 0.62          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 8        | 0.62          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 14       | 0.62          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 19       | 0.62          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 6        | 0.62          |
| (1,472) | 1:662:A:LYS:HA   | 1:665:A:GLU:HB2  | 15       | 0.62          |
| (1,457) | 1:608:A:VAL:HG23 | 1:605:A:HIS:HA   | 11       | 0.62          |
| (1,452) | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 1        | 0.62          |
| (1,396) | 1:664:A:LEU:HD22 | 1:664:A:LEU:HB2  | 10       | 0.62          |
| (1,396) | 1:664:A:LEU:HD23 | 1:664:A:LEU:HB2  | 16       | 0.62          |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD23 | 1        | 0.62          |
| (1,354) | 1:660:A:ILE:HD13 | 1:657:A:ILE:HA   | 5        | 0.62          |
| (1,332) | 1:632:A:ALA:HB2  | 1:611:A:ILE:HD12 | 16       | 0.62          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 4        | 0.62          |
| (1,212) | 1:611:A:ILE:HD11 | 1:607:A:LEU:HD21 | 15       | 0.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,212)  | 1:611:A:ILE:HD12 | 1:607:A:LEU:HD21 | 15       | 0.62          |
| (1,212)  | 1:611:A:ILE:HD13 | 1:607:A:LEU:HD21 | 15       | 0.62          |
| (1,207)  | 1:632:A:ALA:HA   | 1:607:A:LEU:HD12 | 20       | 0.62          |
| (1,163)  | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 3        | 0.62          |
| (1,163)  | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 13       | 0.62          |
| (1,163)  | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 15       | 0.62          |
| (1,47)   | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 1        | 0.62          |
| (1,47)   | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 2        | 0.62          |
| (1,47)   | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 4        | 0.62          |
| (1,47)   | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 5        | 0.62          |
| (1,47)   | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 6        | 0.62          |
| (1,47)   | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 7        | 0.62          |
| (1,47)   | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 9        | 0.62          |
| (1,47)   | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 16       | 0.62          |
| (1,47)   | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 17       | 0.62          |
| (1,47)   | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 20       | 0.62          |
| (1,30)   | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB1  | 8        | 0.62          |
| (3,19)   | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 15       | 0.61          |
| (3,19)   | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 15       | 0.61          |
| (3,19)   | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 15       | 0.61          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 15       | 0.61          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 15       | 0.61          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 15       | 0.61          |
| (3,4)    | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 10       | 0.61          |
| (3,4)    | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 10       | 0.61          |
| (3,4)    | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 10       | 0.61          |
| (3,4)    | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 10       | 0.61          |
| (3,4)    | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 10       | 0.61          |
| (3,4)    | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 10       | 0.61          |
| (2,260)  | 2:540:B:MET:H    | 2:540:B:MET:HG3  | 9        | 0.61          |
| (2,219)  | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 4        | 0.61          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 10       | 0.61          |
| (1,986)  | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 5        | 0.61          |
| (1,914)  | 1:657:A:ILE:H    | 1:656:A:LYS:HB2  | 10       | 0.61          |
| (1,914)  | 1:657:A:ILE:H    | 1:656:A:LYS:HB2  | 13       | 0.61          |
| (1,879)  | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 16       | 0.61          |
| (1,766)  | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 20       | 0.61          |
| (1,745)  | 1:600:A:ARG:H    | 1:599:A:LEU:HB2  | 3        | 0.61          |
| (1,722)  | 1:609:A:GLN:H    | 1:610:A:ALA:HB3  | 2        | 0.61          |
| (1,719)  | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 7        | 0.61          |
| (1,717)  | 1:610:A:ALA:H    | 1:657:A:ILE:HD12 | 17       | 0.61          |
| (1,717)  | 1:610:A:ALA:H    | 1:657:A:ILE:HD12 | 19       | 0.61          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG21 | 15       | 0.61          |
| (1,610) | 1:599:A:LEU:HD22 | 1:603:A:LEU:HD21 | 3        | 0.61          |
| (1,589) | 1:599:A:LEU:HD23 | 1:599:A:LEU:HB2  | 17       | 0.61          |
| (1,589) | 1:599:A:LEU:HD21 | 1:599:A:LEU:HB2  | 18       | 0.61          |
| (1,540) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD11 | 6        | 0.61          |
| (1,415) | 1:620:A:LEU:HD22 | 1:625:A:MET:HG2  | 16       | 0.61          |
| (1,396) | 1:664:A:LEU:HD23 | 1:664:A:LEU:HB2  | 2        | 0.61          |
| (1,396) | 1:664:A:LEU:HD21 | 1:664:A:LEU:HB2  | 20       | 0.61          |
| (1,384) | 1:614:A:THR:HG22 | 1:614:A:THR:HA   | 3        | 0.61          |
| (1,211) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD13 | 2        | 0.61          |
| (1,209) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD21 | 9        | 0.61          |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 8        | 0.61          |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 10       | 0.61          |
| (1,141) | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE1  | 7        | 0.61          |
| (1,141) | 1:595:A:VAL:HG21 | 1:640:A:TYR:HE2  | 7        | 0.61          |
| (1,47)  | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 8        | 0.61          |
| (1,47)  | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 10       | 0.61          |
| (1,47)  | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 13       | 0.61          |
| (1,47)  | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 19       | 0.61          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 13       | 0.6           |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 13       | 0.6           |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 13       | 0.6           |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 13       | 0.6           |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 13       | 0.6           |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 13       | 0.6           |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 18       | 0.6           |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 18       | 0.6           |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 18       | 0.6           |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 18       | 0.6           |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 18       | 0.6           |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 18       | 0.6           |
| (2,260) | 2:540:B:MET:H    | 2:540:B:MET:HG3  | 13       | 0.6           |
| (2,252) | 2:535:B:SER:H    | 2:534:B:PHE:HD1  | 4        | 0.6           |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 4        | 0.6           |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 9        | 0.6           |
| (2,69)  | 2:534:B:PHE:HA   | 2:534:B:PHE:HD1  | 20       | 0.6           |
| (2,69)  | 2:534:B:PHE:HA   | 2:534:B:PHE:HD2  | 20       | 0.6           |
| (1,986) | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 20       | 0.6           |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG21 | 16       | 0.6           |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG22 | 19       | 0.6           |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 10       | 0.6           |
| (1,745) | 1:600:A:ARG:H    | 1:599:A:LEU:HB2  | 4        | 0.6           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG22 | 4        | 0.6           |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB3  | 6        | 0.6           |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB1  | 12       | 0.6           |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD13 | 20       | 0.6           |
| (1,583) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD12 | 17       | 0.6           |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD23 | 2        | 0.6           |
| (1,495) | 1:653:A:LEU:HD11 | 1:603:A:LEU:HD11 | 11       | 0.6           |
| (1,457) | 1:608:A:VAL:HG23 | 1:605:A:HIS:HA   | 8        | 0.6           |
| (1,452) | 1:668:A:ARG:HB3  | 1:665:A:GLU:HA   | 7        | 0.6           |
| (1,396) | 1:664:A:LEU:HD22 | 1:664:A:LEU:HB2  | 13       | 0.6           |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG13 | 2        | 0.6           |
| (1,354) | 1:660:A:ILE:HD11 | 1:657:A:ILE:HA   | 14       | 0.6           |
| (1,354) | 1:660:A:ILE:HD11 | 1:657:A:ILE:HA   | 18       | 0.6           |
| (1,332) | 1:632:A:ALA:HB1  | 1:611:A:ILE:HD13 | 12       | 0.6           |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG21 | 17       | 0.6           |
| (1,225) | 1:632:A:ALA:HB1  | 1:604:A:VAL:HG21 | 8        | 0.6           |
| (1,212) | 1:611:A:ILE:HD11 | 1:607:A:LEU:HD21 | 17       | 0.6           |
| (1,212) | 1:611:A:ILE:HD12 | 1:607:A:LEU:HD21 | 17       | 0.6           |
| (1,212) | 1:611:A:ILE:HD13 | 1:607:A:LEU:HD21 | 17       | 0.6           |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 9        | 0.6           |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 16       | 0.6           |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 17       | 0.6           |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 6        | 0.59          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 6        | 0.59          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 6        | 0.59          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 6        | 0.59          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 6        | 0.59          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 6        | 0.59          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 19       | 0.59          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 19       | 0.59          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 19       | 0.59          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 19       | 0.59          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 19       | 0.59          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 19       | 0.59          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 2        | 0.59          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 2        | 0.59          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 2        | 0.59          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 2        | 0.59          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 2        | 0.59          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 2        | 0.59          |
| (2,260) | 2:540:B:MET:H    | 2:540:B:MET:HG3  | 16       | 0.59          |
| (2,260) | 2:540:B:MET:H    | 2:540:B:MET:HG3  | 19       | 0.59          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 1        | 0.59          |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 1        | 0.59          |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 1        | 0.59          |
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 13       | 0.59          |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 13       | 0.59          |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 13       | 0.59          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD11 | 13       | 0.59          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD12 | 13       | 0.59          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD13 | 13       | 0.59          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD11 | 13       | 0.59          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD12 | 13       | 0.59          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD13 | 13       | 0.59          |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 4        | 0.59          |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 15       | 0.59          |
| (1,875) | 1:645:A:SER:H    | 1:648:A:GLU:HB2  | 7        | 0.59          |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 20       | 0.59          |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG21 | 3        | 0.59          |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG21 | 18       | 0.59          |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG23 | 2        | 0.59          |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB1  | 1        | 0.59          |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB1  | 8        | 0.59          |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD12 | 11       | 0.59          |
| (1,580) | 1:599:A:LEU:HD11 | 1:599:A:LEU:HA   | 5        | 0.59          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD21 | 2        | 0.59          |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD22 | 14       | 0.59          |
| (1,492) | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 14       | 0.59          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 17       | 0.59          |
| (1,411) | 1:629:A:VAL:HG11 | 1:630:A:ALA:HB1  | 14       | 0.59          |
| (1,396) | 1:664:A:LEU:HD23 | 1:664:A:LEU:HB2  | 11       | 0.59          |
| (1,380) | 1:620:A:LEU:HD13 | 1:617:A:PRO:HA   | 7        | 0.59          |
| (1,275) | 1:593:A:GLU:HB3  | 1:593:A:GLU:HG2  | 3        | 0.59          |
| (1,275) | 1:593:A:GLU:HB3  | 1:593:A:GLU:HG2  | 15       | 0.59          |
| (1,275) | 1:593:A:GLU:HB3  | 1:593:A:GLU:HG2  | 18       | 0.59          |
| (1,275) | 1:593:A:GLU:HB3  | 1:593:A:GLU:HG2  | 20       | 0.59          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG23 | 16       | 0.59          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG21 | 18       | 0.59          |
| (1,212) | 1:611:A:ILE:HD11 | 1:607:A:LEU:HD22 | 16       | 0.59          |
| (1,212) | 1:611:A:ILE:HD12 | 1:607:A:LEU:HD22 | 16       | 0.59          |
| (1,212) | 1:611:A:ILE:HD13 | 1:607:A:LEU:HD22 | 16       | 0.59          |
| (1,207) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD12 | 2        | 0.59          |
| (1,47)  | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 3        | 0.59          |
| (1,47)  | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 11       | 0.59          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,47)  | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 12       | 0.59          |
| (1,47)  | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 14       | 0.59          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 18       | 0.59          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 3        | 0.58          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 3        | 0.58          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 3        | 0.58          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 3        | 0.58          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 3        | 0.58          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 3        | 0.58          |
| (2,260) | 2:540:B:MET:H    | 2:540:B:MET:HG3  | 14       | 0.58          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 1        | 0.58          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 2        | 0.58          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 10       | 0.58          |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 13       | 0.58          |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG23 | 14       | 0.58          |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 16       | 0.58          |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG23 | 11       | 0.58          |
| (1,745) | 1:600:A:ARG:H    | 1:599:A:LEU:HB2  | 7        | 0.58          |
| (1,745) | 1:600:A:ARG:H    | 1:599:A:LEU:HB2  | 20       | 0.58          |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB2  | 5        | 0.58          |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB1  | 13       | 0.58          |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB2  | 14       | 0.58          |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD12 | 9        | 0.58          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG23 | 18       | 0.58          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD11 | 20       | 0.58          |
| (1,659) | 1:652:A:LEU:HB3  | 1:639:A:MET:HE3  | 6        | 0.58          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD11 | 12       | 0.58          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD11 | 12       | 0.58          |
| (1,610) | 1:599:A:LEU:HD23 | 1:603:A:LEU:HD21 | 9        | 0.58          |
| (1,548) | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 7        | 0.58          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD23 | 7        | 0.58          |
| (1,465) | 1:589:A:LYS:HG2  | 1:589:A:LYS:HE2  | 20       | 0.58          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 9        | 0.58          |
| (1,457) | 1:608:A:VAL:HG22 | 1:605:A:HIS:HA   | 15       | 0.58          |
| (1,453) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HA   | 3        | 0.58          |
| (1,453) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HA   | 17       | 0.58          |
| (1,453) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HA   | 19       | 0.58          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 12       | 0.58          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 15       | 0.58          |
| (1,275) | 1:593:A:GLU:HB3  | 1:593:A:GLU:HG2  | 1        | 0.58          |
| (1,229) | 1:636:A:GLU:HG2  | 1:604:A:VAL:HG21 | 17       | 0.58          |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 5        | 0.58          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,47)   | 1:597:A:GLN:HG2  | 1:597:A:GLN:HB2  | 18       | 0.58          |
| (3,29)   | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 9        | 0.57          |
| (3,29)   | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 9        | 0.57          |
| (3,24)   | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 8        | 0.57          |
| (3,24)   | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 8        | 0.57          |
| (3,24)   | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 8        | 0.57          |
| (3,24)   | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 8        | 0.57          |
| (3,24)   | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 8        | 0.57          |
| (3,24)   | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 8        | 0.57          |
| (3,24)   | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 8        | 0.57          |
| (3,24)   | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 8        | 0.57          |
| (3,24)   | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 8        | 0.57          |
| (3,24)   | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 15       | 0.57          |
| (3,24)   | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 15       | 0.57          |
| (3,24)   | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 15       | 0.57          |
| (3,24)   | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 15       | 0.57          |
| (3,24)   | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 15       | 0.57          |
| (3,24)   | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 15       | 0.57          |
| (3,24)   | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 15       | 0.57          |
| (3,24)   | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 15       | 0.57          |
| (3,24)   | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 15       | 0.57          |
| (2,252)  | 2:535:B:SER:H    | 2:534:B:PHE:HD1  | 17       | 0.57          |
| (2,219)  | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 6        | 0.57          |
| (2,135)  | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 4        | 0.57          |
| (2,135)  | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 4        | 0.57          |
| (2,135)  | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 4        | 0.57          |
| (2,76)   | 2:542:B:PHE:HA   | 2:542:B:PHE:HD1  | 7        | 0.57          |
| (2,76)   | 2:542:B:PHE:HA   | 2:542:B:PHE:HD2  | 7        | 0.57          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG11 | 7        | 0.57          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG12 | 7        | 0.57          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG13 | 7        | 0.57          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG11 | 7        | 0.57          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG12 | 7        | 0.57          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG13 | 7        | 0.57          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG11 | 7        | 0.57          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG12 | 7        | 0.57          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG13 | 7        | 0.57          |
| (1,986)  | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 15       | 0.57          |
| (1,935)  | 1:663:A:GLU:H    | 1:663:A:GLU:HG2  | 13       | 0.57          |
| (1,935)  | 1:663:A:GLU:H    | 1:663:A:GLU:HG2  | 20       | 0.57          |
| (1,879)  | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 1        | 0.57          |
| (1,879)  | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 2        | 0.57          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 17       | 0.57          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG22 | 2        | 0.57          |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB3  | 4        | 0.57          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG23 | 8        | 0.57          |
| (1,659) | 1:652:A:LEU:HB3  | 1:639:A:MET:HE1  | 9        | 0.57          |
| (1,657) | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE1  | 14       | 0.57          |
| (1,657) | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE2  | 14       | 0.57          |
| (1,572) | 1:654:A:ALA:HB1  | 1:657:A:ILE:HD13 | 17       | 0.57          |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD23 | 12       | 0.57          |
| (1,495) | 1:653:A:LEU:HD11 | 1:603:A:LEU:HD11 | 7        | 0.57          |
| (1,465) | 1:589:A:LYS:HG2  | 1:589:A:LYS:HE2  | 11       | 0.57          |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 6        | 0.57          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 7        | 0.57          |
| (1,275) | 1:593:A:GLU:HB3  | 1:593:A:GLU:HG2  | 19       | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 1        | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 3        | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 5        | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 6        | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 8        | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 9        | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 10       | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 12       | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 13       | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 15       | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 16       | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 18       | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 19       | 0.57          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 20       | 0.57          |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG23 | 6        | 0.57          |
| (1,172) | 1:651:A:HIS:HB2  | 1:651:A:HIS:HD2  | 8        | 0.57          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 5        | 0.56          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 5        | 0.56          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 5        | 0.56          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 5        | 0.56          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 5        | 0.56          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 5        | 0.56          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 19       | 0.56          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 19       | 0.56          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 19       | 0.56          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 19       | 0.56          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 19       | 0.56          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 19       | 0.56          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,219) | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 7        | 0.56          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD1  | 7        | 0.56          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD2  | 7        | 0.56          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD1  | 7        | 0.56          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD2  | 7        | 0.56          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD1  | 7        | 0.56          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD2  | 7        | 0.56          |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 1        | 0.56          |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 7        | 0.56          |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 18       | 0.56          |
| (1,819) | 1:598:A:ASP:H    | 1:596:A:THR:HG21 | 15       | 0.56          |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 2        | 0.56          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 14       | 0.56          |
| (1,745) | 1:600:A:ARG:H    | 1:599:A:LEU:HB2  | 8        | 0.56          |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB3  | 18       | 0.56          |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD12 | 1        | 0.56          |
| (1,711) | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 13       | 0.56          |
| (1,711) | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 17       | 0.56          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG22 | 6        | 0.56          |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 1        | 0.56          |
| (1,655) | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 3        | 0.56          |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD22 | 5        | 0.56          |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD23 | 18       | 0.56          |
| (1,606) | 1:595:A:VAL:HA   | 1:599:A:LEU:HD23 | 9        | 0.56          |
| (1,392) | 1:635:A:VAL:HG21 | 1:632:A:ALA:HA   | 20       | 0.56          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB3  | 15       | 0.56          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 17       | 0.56          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG23 | 15       | 0.56          |
| (1,221) | 1:607:A:LEU:HB3  | 1:604:A:VAL:HA   | 6        | 0.56          |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 11       | 0.56          |
| (1,95)  | 1:662:A:LYS:HD2  | 1:662:A:LYS:HE2  | 4        | 0.56          |
| (1,2)   | 1:639:A:MET:HG2  | 1:639:A:MET:HE3  | 11       | 0.56          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 11       | 0.55          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 11       | 0.55          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 11       | 0.55          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 11       | 0.55          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 11       | 0.55          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 11       | 0.55          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 11       | 0.55          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 11       | 0.55          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 17       | 0.55          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 17       | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,19)   | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 17       | 0.55          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 17       | 0.55          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 17       | 0.55          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 17       | 0.55          |
| (2,219)  | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 3        | 0.55          |
| (2,135)  | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 12       | 0.55          |
| (2,135)  | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 12       | 0.55          |
| (2,135)  | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 12       | 0.55          |
| (2,133)  | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 12       | 0.55          |
| (2,133)  | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 13       | 0.55          |
| (2,132)  | 2:546:B:LEU:HB2  | 2:543:B:SER:HA   | 10       | 0.55          |
| (2,132)  | 2:546:B:LEU:HB2  | 2:543:B:SER:HA   | 16       | 0.55          |
| (2,109)  | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 16       | 0.55          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 13       | 0.55          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 13       | 0.55          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 13       | 0.55          |
| (1,945)  | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 8        | 0.55          |
| (1,945)  | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 9        | 0.55          |
| (1,925)  | 1:660:A:ILE:H    | 1:660:A:ILE:HD13 | 13       | 0.55          |
| (1,879)  | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 5        | 0.55          |
| (1,846)  | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 15       | 0.55          |
| (1,813)  | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 3        | 0.55          |
| (1,813)  | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 5        | 0.55          |
| (1,813)  | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 18       | 0.55          |
| (1,722)  | 1:609:A:GLN:H    | 1:610:A:ALA:HB2  | 3        | 0.55          |
| (1,711)  | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 4        | 0.55          |
| (1,658)  | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG21 | 5        | 0.55          |
| (1,655)  | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 2        | 0.55          |
| (1,655)  | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 4        | 0.55          |
| (1,655)  | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 6        | 0.55          |
| (1,655)  | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 7        | 0.55          |
| (1,655)  | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 9        | 0.55          |
| (1,655)  | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 13       | 0.55          |
| (1,655)  | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 19       | 0.55          |
| (1,640)  | 1:639:A:MET:HB3  | 1:653:A:LEU:HD13 | 6        | 0.55          |
| (1,636)  | 1:639:A:MET:HE2  | 1:639:A:MET:HA   | 3        | 0.55          |
| (1,601)  | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD1  | 9        | 0.55          |
| (1,601)  | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD2  | 9        | 0.55          |
| (1,598)  | 1:595:A:VAL:HG21 | 1:592:A:HIS:HA   | 13       | 0.55          |
| (1,583)  | 1:603:A:LEU:HD11 | 1:599:A:LEU:HD13 | 12       | 0.55          |
| (1,513)  | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 20       | 0.55          |
| (1,479)  | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 16       | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,457)  | 1:608:A:VAL:HG22 | 1:605:A:HIS:HA   | 14       | 0.55          |
| (1,453)  | 1:634:A:LYS:HG2  | 1:634:A:LYS:HA   | 18       | 0.55          |
| (1,424)  | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 15       | 0.55          |
| (1,366)  | 1:639:A:MET:HE3  | 1:653:A:LEU:HD22 | 7        | 0.55          |
| (1,256)  | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 14       | 0.55          |
| (1,200)  | 1:619:A:ALA:HB3  | 1:620:A:LEU:HA   | 12       | 0.55          |
| (1,95)   | 1:662:A:LYS:HD2  | 1:662:A:LYS:HE2  | 12       | 0.55          |
| (1,65)   | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 1        | 0.55          |
| (1,2)    | 1:639:A:MET:HG2  | 1:639:A:MET:HE2  | 8        | 0.55          |
| (3,34)   | 1:664:A:LEU:HD21 | 2:542:B:PHE:HE1  | 14       | 0.54          |
| (3,34)   | 1:664:A:LEU:HD21 | 2:542:B:PHE:HE2  | 14       | 0.54          |
| (3,34)   | 1:664:A:LEU:HD22 | 2:542:B:PHE:HE1  | 14       | 0.54          |
| (3,34)   | 1:664:A:LEU:HD22 | 2:542:B:PHE:HE2  | 14       | 0.54          |
| (3,34)   | 1:664:A:LEU:HD23 | 2:542:B:PHE:HE1  | 14       | 0.54          |
| (3,34)   | 1:664:A:LEU:HD23 | 2:542:B:PHE:HE2  | 14       | 0.54          |
| (3,29)   | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 18       | 0.54          |
| (3,29)   | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 18       | 0.54          |
| (3,19)   | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 18       | 0.54          |
| (3,19)   | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 18       | 0.54          |
| (3,19)   | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 18       | 0.54          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 18       | 0.54          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 18       | 0.54          |
| (3,19)   | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 18       | 0.54          |
| (2,169)  | 2:544:B:ALA:HA   | 2:547:B:SER:HB3  | 14       | 0.54          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD1  | 1        | 0.54          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD2  | 1        | 0.54          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD1  | 1        | 0.54          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD2  | 1        | 0.54          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD1  | 1        | 0.54          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD2  | 1        | 0.54          |
| (1,935)  | 1:663:A:GLU:H    | 1:663:A:GLU:HG2  | 10       | 0.54          |
| (1,879)  | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 3        | 0.54          |
| (1,879)  | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 13       | 0.54          |
| (1,846)  | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 8        | 0.54          |
| (1,813)  | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 1        | 0.54          |
| (1,813)  | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 7        | 0.54          |
| (1,762)  | 1:605:A:HIS:H    | 1:604:A:VAL:HG23 | 6        | 0.54          |
| (1,722)  | 1:609:A:GLN:H    | 1:610:A:ALA:HB1  | 16       | 0.54          |
| (1,722)  | 1:609:A:GLN:H    | 1:610:A:ALA:HB1  | 20       | 0.54          |
| (1,673)  | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 5        | 0.54          |
| (1,673)  | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 12       | 0.54          |
| (1,658)  | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG22 | 4        | 0.54          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,655) | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 1        | 0.54          |
| (1,655) | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 8        | 0.54          |
| (1,655) | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 11       | 0.54          |
| (1,655) | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 12       | 0.54          |
| (1,655) | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 14       | 0.54          |
| (1,655) | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 15       | 0.54          |
| (1,655) | 1:623:A:ARG:HB2  | 1:623:A:ARG:HA   | 16       | 0.54          |
| (1,610) | 1:599:A:LEU:HD21 | 1:603:A:LEU:HD22 | 4        | 0.54          |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD23 | 1        | 0.54          |
| (1,513) | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 16       | 0.54          |
| (1,483) | 1:667:A:LYS:HA   | 1:667:A:LYS:HG3  | 2        | 0.54          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 4        | 0.54          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 3        | 0.54          |
| (1,453) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HA   | 16       | 0.54          |
| (1,434) | 1:635:A:VAL:HG23 | 1:639:A:MET:HE3  | 10       | 0.54          |
| (1,292) | 1:633:A:LYS:HG2  | 1:633:A:LYS:HA   | 19       | 0.54          |
| (1,263) | 1:607:A:LEU:HD21 | 1:632:A:ALA:HB1  | 1        | 0.54          |
| (1,211) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD13 | 20       | 0.54          |
| (1,200) | 1:619:A:ALA:HB3  | 1:620:A:LEU:HA   | 10       | 0.54          |
| (1,200) | 1:619:A:ALA:HB1  | 1:620:A:LEU:HA   | 18       | 0.54          |
| (1,172) | 1:651:A:HIS:HB2  | 1:651:A:HIS:HD2  | 17       | 0.54          |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 16       | 0.54          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD1  | 12       | 0.54          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD2  | 12       | 0.54          |
| (1,95)  | 1:662:A:LYS:HD2  | 1:662:A:LYS:HE2  | 3        | 0.54          |
| (1,95)  | 1:662:A:LYS:HD2  | 1:662:A:LYS:HE2  | 8        | 0.54          |
| (1,95)  | 1:662:A:LYS:HD2  | 1:662:A:LYS:HE2  | 9        | 0.54          |
| (1,95)  | 1:662:A:LYS:HD2  | 1:662:A:LYS:HE2  | 13       | 0.54          |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 15       | 0.54          |
| (1,36)  | 1:609:A:GLN:HA   | 1:609:A:GLN:HG3  | 15       | 0.54          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 1        | 0.54          |
| (1,6)   | 1:608:A:VAL:HG11 | 1:625:A:MET:HE3  | 8        | 0.54          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 19       | 0.53          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 19       | 0.53          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 6        | 0.53          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 6        | 0.53          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 8        | 0.53          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 8        | 0.53          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 8        | 0.53          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 8        | 0.53          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 8        | 0.53          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 8        | 0.53          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,267) | 2:542:B:PHE:H    | 2:540:B:MET:HB2  | 13       | 0.53          |
| (2,219) | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 16       | 0.53          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 6        | 0.53          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 18       | 0.53          |
| (2,132) | 2:546:B:LEU:HB2  | 2:543:B:SER:HA   | 4        | 0.53          |
| (2,69)  | 2:534:B:PHE:HA   | 2:534:B:PHE:HD1  | 19       | 0.53          |
| (2,69)  | 2:534:B:PHE:HA   | 2:534:B:PHE:HD2  | 19       | 0.53          |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 5        | 0.53          |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 18       | 0.53          |
| (1,915) | 1:657:A:ILE:H    | 1:657:A:ILE:HD12 | 3        | 0.53          |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 1        | 0.53          |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 16       | 0.53          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 9        | 0.53          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG22 | 16       | 0.53          |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB3  | 9        | 0.53          |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB3  | 19       | 0.53          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG21 | 7        | 0.53          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG23 | 12       | 0.53          |
| (1,701) | 1:614:A:THR:H    | 1:614:A:THR:HG23 | 16       | 0.53          |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 4        | 0.53          |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 7        | 0.53          |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 14       | 0.53          |
| (1,598) | 1:595:A:VAL:HG22 | 1:592:A:HIS:HA   | 9        | 0.53          |
| (1,598) | 1:595:A:VAL:HG23 | 1:592:A:HIS:HA   | 11       | 0.53          |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD13 | 18       | 0.53          |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD13 | 18       | 0.53          |
| (1,534) | 1:639:A:MET:HG2  | 1:653:A:LEU:HD21 | 14       | 0.53          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 3        | 0.53          |
| (1,450) | 1:665:A:GLU:HA   | 1:665:A:GLU:HG2  | 12       | 0.53          |
| (1,435) | 1:653:A:LEU:HD11 | 1:639:A:MET:HE2  | 16       | 0.53          |
| (1,423) | 1:629:A:VAL:HG13 | 1:626:A:GLU:HG2  | 1        | 0.53          |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG13 | 6        | 0.53          |
| (1,358) | 1:620:A:LEU:HD22 | 1:620:A:LEU:HB2  | 11       | 0.53          |
| (1,332) | 1:632:A:ALA:HB3  | 1:611:A:ILE:HD11 | 10       | 0.53          |
| (1,211) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD13 | 15       | 0.53          |
| (1,200) | 1:619:A:ALA:HB3  | 1:620:A:LEU:HA   | 2        | 0.53          |
| (1,200) | 1:619:A:ALA:HB1  | 1:620:A:LEU:HA   | 9        | 0.53          |
| (1,200) | 1:619:A:ALA:HB1  | 1:620:A:LEU:HA   | 11       | 0.53          |
| (1,200) | 1:619:A:ALA:HB1  | 1:620:A:LEU:HA   | 13       | 0.53          |
| (1,200) | 1:619:A:ALA:HB1  | 1:620:A:LEU:HA   | 15       | 0.53          |
| (1,200) | 1:619:A:ALA:HB1  | 1:620:A:LEU:HA   | 19       | 0.53          |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 10       | 0.53          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,33)  | 1:664:A:LEU:HD21 | 2:538:B:ALA:HA   | 7        | 0.52          |
| (3,33)  | 1:664:A:LEU:HD22 | 2:538:B:ALA:HA   | 7        | 0.52          |
| (3,33)  | 1:664:A:LEU:HD23 | 2:538:B:ALA:HA   | 7        | 0.52          |
| (2,267) | 2:542:B:PHE:H    | 2:540:B:MET:HB2  | 19       | 0.52          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG22 | 2        | 0.52          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 5        | 0.52          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 17       | 0.52          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 5        | 0.52          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 8        | 0.52          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 13       | 0.52          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 20       | 0.52          |
| (2,135) | 2:544:B:ALA:HB1  | 2:543:B:SER:HB3  | 20       | 0.52          |
| (2,135) | 2:544:B:ALA:HB2  | 2:543:B:SER:HB3  | 20       | 0.52          |
| (2,135) | 2:544:B:ALA:HB3  | 2:543:B:SER:HB3  | 20       | 0.52          |
| (2,95)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HB3  | 15       | 0.52          |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 14       | 0.52          |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 20       | 0.52          |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB3  | 11       | 0.52          |
| (1,745) | 1:600:A:ARG:H    | 1:599:A:LEU:HB2  | 12       | 0.52          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG22 | 11       | 0.52          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG21 | 14       | 0.52          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG22 | 20       | 0.52          |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 6        | 0.52          |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 8        | 0.52          |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 9        | 0.52          |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 11       | 0.52          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD12 | 12       | 0.52          |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG23 | 9        | 0.52          |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD12 | 4        | 0.52          |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD13 | 5        | 0.52          |
| (1,636) | 1:639:A:MET:HE2  | 1:639:A:MET:HA   | 14       | 0.52          |
| (1,636) | 1:639:A:MET:HE3  | 1:639:A:MET:HA   | 20       | 0.52          |
| (1,594) | 1:634:A:LYS:HG2  | 1:635:A:VAL:HG12 | 10       | 0.52          |
| (1,524) | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD3  | 7        | 0.52          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 5        | 0.52          |
| (1,457) | 1:608:A:VAL:HG23 | 1:605:A:HIS:HA   | 2        | 0.52          |
| (1,453) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HA   | 2        | 0.52          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG22 | 18       | 0.52          |
| (1,358) | 1:620:A:LEU:HD22 | 1:620:A:LEU:HB2  | 4        | 0.52          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG13 | 18       | 0.52          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG22 | 6        | 0.52          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG22 | 11       | 0.52          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,200) | 1:619:A:ALA:HB1  | 1:620:A:LEU:HA   | 1        | 0.52          |
| (1,200) | 1:619:A:ALA:HB1  | 1:620:A:LEU:HA   | 4        | 0.52          |
| (1,200) | 1:619:A:ALA:HB3  | 1:620:A:LEU:HA   | 16       | 0.52          |
| (1,200) | 1:619:A:ALA:HB1  | 1:620:A:LEU:HA   | 17       | 0.52          |
| (1,200) | 1:619:A:ALA:HB3  | 1:620:A:LEU:HA   | 20       | 0.52          |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE1  | 18       | 0.52          |
| (1,148) | 1:635:A:VAL:HG13 | 1:631:A:TYR:HE2  | 18       | 0.52          |
| (1,84)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HG2  | 1        | 0.52          |
| (1,36)  | 1:609:A:GLN:HA   | 1:609:A:GLN:HG3  | 7        | 0.52          |
| (1,3)   | 1:639:A:MET:HG3  | 1:639:A:MET:HE3  | 14       | 0.52          |
| (1,2)   | 1:639:A:MET:HG2  | 1:639:A:MET:HE2  | 17       | 0.52          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 8        | 0.51          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 8        | 0.51          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 8        | 0.51          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 8        | 0.51          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 8        | 0.51          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 8        | 0.51          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 13       | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 1        | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 2        | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 3        | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 4        | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 6        | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 9        | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 10       | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 11       | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 12       | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 14       | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 15       | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 16       | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 17       | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 18       | 0.51          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 19       | 0.51          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD11 | 4        | 0.51          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD12 | 4        | 0.51          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD13 | 4        | 0.51          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD11 | 4        | 0.51          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD12 | 4        | 0.51          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD13 | 4        | 0.51          |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD13 | 10       | 0.51          |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 10       | 0.51          |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 17       | 0.51          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,843) | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 3        | 0.51          |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB3  | 14       | 0.51          |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 8        | 0.51          |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 17       | 0.51          |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 19       | 0.51          |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 20       | 0.51          |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG23 | 20       | 0.51          |
| (1,724) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HD2  | 14       | 0.51          |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB3  | 10       | 0.51          |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 16       | 0.51          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD11 | 10       | 0.51          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD11 | 10       | 0.51          |
| (1,572) | 1:654:A:ALA:HB2  | 1:657:A:ILE:HD11 | 14       | 0.51          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 16       | 0.51          |
| (1,453) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HA   | 4        | 0.51          |
| (1,424) | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 17       | 0.51          |
| (1,358) | 1:620:A:LEU:HD21 | 1:620:A:LEU:HB2  | 3        | 0.51          |
| (1,358) | 1:620:A:LEU:HD23 | 1:620:A:LEU:HB2  | 9        | 0.51          |
| (1,358) | 1:620:A:LEU:HD22 | 1:620:A:LEU:HB2  | 12       | 0.51          |
| (1,358) | 1:620:A:LEU:HD22 | 1:620:A:LEU:HB2  | 13       | 0.51          |
| (1,358) | 1:620:A:LEU:HD21 | 1:620:A:LEU:HB2  | 14       | 0.51          |
| (1,358) | 1:620:A:LEU:HD23 | 1:620:A:LEU:HB2  | 20       | 0.51          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB3  | 14       | 0.51          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG22 | 7        | 0.51          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG22 | 12       | 0.51          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG22 | 20       | 0.51          |
| (1,221) | 1:607:A:LEU:HB3  | 1:604:A:VAL:HA   | 4        | 0.51          |
| (1,210) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD21 | 5        | 0.51          |
| (1,200) | 1:619:A:ALA:HB1  | 1:620:A:LEU:HA   | 5        | 0.51          |
| (1,200) | 1:619:A:ALA:HB1  | 1:620:A:LEU:HA   | 6        | 0.51          |
| (1,200) | 1:619:A:ALA:HB2  | 1:620:A:LEU:HA   | 7        | 0.51          |
| (1,200) | 1:619:A:ALA:HB3  | 1:620:A:LEU:HA   | 8        | 0.51          |
| (1,200) | 1:619:A:ALA:HB3  | 1:620:A:LEU:HA   | 14       | 0.51          |
| (1,84)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HG2  | 7        | 0.51          |
| (1,13)  | 1:617:A:PRO:HD2  | 1:616:A:ASP:HB3  | 10       | 0.51          |
| (1,2)   | 1:639:A:MET:HG2  | 1:639:A:MET:HE1  | 7        | 0.51          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 14       | 0.5           |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 14       | 0.5           |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 14       | 0.5           |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 14       | 0.5           |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 14       | 0.5           |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 14       | 0.5           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 16       | 0.5           |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 16       | 0.5           |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 16       | 0.5           |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 16       | 0.5           |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 16       | 0.5           |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 16       | 0.5           |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 16       | 0.5           |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 16       | 0.5           |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 16       | 0.5           |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG22 | 20       | 0.5           |
| (1,942) | 1:664:A:LEU:H    | 1:664:A:LEU:HD12 | 17       | 0.5           |
| (1,903) | 1:653:A:LEU:H    | 1:653:A:LEU:HD13 | 14       | 0.5           |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB1  | 9        | 0.5           |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB1  | 10       | 0.5           |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB2  | 13       | 0.5           |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 9        | 0.5           |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 12       | 0.5           |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG21 | 9        | 0.5           |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG21 | 13       | 0.5           |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG22 | 18       | 0.5           |
| (1,724) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HD2  | 13       | 0.5           |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB1  | 15       | 0.5           |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 19       | 0.5           |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 20       | 0.5           |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD11 | 3        | 0.5           |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD11 | 14       | 0.5           |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD22 | 17       | 0.5           |
| (1,601) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD1  | 1        | 0.5           |
| (1,601) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD2  | 1        | 0.5           |
| (1,601) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD1  | 2        | 0.5           |
| (1,601) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD2  | 2        | 0.5           |
| (1,503) | 1:625:A:MET:HG2  | 1:629:A:VAL:HG23 | 17       | 0.5           |
| (1,453) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HA   | 14       | 0.5           |
| (1,424) | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 6        | 0.5           |
| (1,424) | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 9        | 0.5           |
| (1,411) | 1:629:A:VAL:HG11 | 1:630:A:ALA:HB1  | 19       | 0.5           |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG12 | 17       | 0.5           |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG21 | 12       | 0.5           |
| (1,358) | 1:620:A:LEU:HD21 | 1:620:A:LEU:HB2  | 5        | 0.5           |
| (1,358) | 1:620:A:LEU:HD23 | 1:620:A:LEU:HB2  | 8        | 0.5           |
| (1,358) | 1:620:A:LEU:HD22 | 1:620:A:LEU:HB2  | 16       | 0.5           |
| (1,358) | 1:620:A:LEU:HD21 | 1:620:A:LEU:HB2  | 18       | 0.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,357)  | 1:608:A:VAL:HG22 | 1:629:A:VAL:HA   | 20       | 0.5           |
| (1,143)  | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 9        | 0.5           |
| (1,143)  | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 9        | 0.5           |
| (1,99)   | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 12       | 0.5           |
| (3,12)   | 1:625:A:MET:HA   | 2:545:B:LEU:HD11 | 20       | 0.49          |
| (3,12)   | 1:625:A:MET:HA   | 2:545:B:LEU:HD12 | 20       | 0.49          |
| (3,12)   | 1:625:A:MET:HA   | 2:545:B:LEU:HD13 | 20       | 0.49          |
| (3,4)    | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 9        | 0.49          |
| (3,4)    | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 9        | 0.49          |
| (3,4)    | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 9        | 0.49          |
| (3,4)    | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 9        | 0.49          |
| (3,4)    | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 9        | 0.49          |
| (3,4)    | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 9        | 0.49          |
| (2,267)  | 2:542:B:PHE:H    | 2:540:B:MET:HB2  | 9        | 0.49          |
| (2,267)  | 2:542:B:PHE:H    | 2:540:B:MET:HB2  | 16       | 0.49          |
| (2,219)  | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 12       | 0.49          |
| (2,214)  | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 11       | 0.49          |
| (2,109)  | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 6        | 0.49          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 6        | 0.49          |
| (1,951)  | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 6        | 0.49          |
| (1,951)  | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 13       | 0.49          |
| (1,951)  | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 15       | 0.49          |
| (1,942)  | 1:664:A:LEU:H    | 1:664:A:LEU:HD13 | 15       | 0.49          |
| (1,935)  | 1:663:A:GLU:H    | 1:663:A:GLU:HG2  | 6        | 0.49          |
| (1,935)  | 1:663:A:GLU:H    | 1:663:A:GLU:HG2  | 14       | 0.49          |
| (1,925)  | 1:660:A:ILE:H    | 1:660:A:ILE:HD12 | 19       | 0.49          |
| (1,824)  | 1:628:A:LEU:H    | 1:630:A:ALA:HB1  | 4        | 0.49          |
| (1,824)  | 1:628:A:LEU:H    | 1:630:A:ALA:HB3  | 12       | 0.49          |
| (1,762)  | 1:605:A:HIS:H    | 1:604:A:VAL:HG21 | 15       | 0.49          |
| (1,762)  | 1:605:A:HIS:H    | 1:604:A:VAL:HG23 | 16       | 0.49          |
| (1,745)  | 1:600:A:ARG:H    | 1:599:A:LEU:HB2  | 2        | 0.49          |
| (1,743)  | 1:599:A:LEU:H    | 1:596:A:THR:HG21 | 12       | 0.49          |
| (1,711)  | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 3        | 0.49          |
| (1,710)  | 1:588:A:ARG:H    | 1:587:A:VAL:HG22 | 5        | 0.49          |
| (1,673)  | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 2        | 0.49          |
| (1,673)  | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 3        | 0.49          |
| (1,673)  | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 15       | 0.49          |
| (1,673)  | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 17       | 0.49          |
| (1,670)  | 1:620:A:LEU:H    | 1:620:A:LEU:HD12 | 5        | 0.49          |
| (1,658)  | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG23 | 7        | 0.49          |
| (1,657)  | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE1  | 12       | 0.49          |
| (1,657)  | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE2  | 12       | 0.49          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD11 | 1        | 0.49          |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD13 | 9        | 0.49          |
| (1,598) | 1:595:A:VAL:HG23 | 1:592:A:HIS:HA   | 6        | 0.49          |
| (1,571) | 1:591:A:TRP:HD1  | 1:589:A:LYS:HA   | 1        | 0.49          |
| (1,469) | 1:635:A:VAL:HA   | 1:635:A:VAL:HG11 | 15       | 0.49          |
| (1,453) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HA   | 9        | 0.49          |
| (1,392) | 1:635:A:VAL:HG22 | 1:632:A:ALA:HA   | 13       | 0.49          |
| (1,358) | 1:620:A:LEU:HD21 | 1:620:A:LEU:HB2  | 17       | 0.49          |
| (1,302) | 1:614:A:THR:HG22 | 1:617:A:PRO:HA   | 13       | 0.49          |
| (1,225) | 1:632:A:ALA:HB3  | 1:604:A:VAL:HG23 | 3        | 0.49          |
| (1,211) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD12 | 8        | 0.49          |
| (1,200) | 1:619:A:ALA:HB3  | 1:620:A:LEU:HA   | 3        | 0.49          |
| (1,96)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HD3  | 10       | 0.49          |
| (1,96)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HD3  | 13       | 0.49          |
| (1,96)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HD3  | 18       | 0.49          |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB1  | 18       | 0.49          |
| (1,3)   | 1:639:A:MET:HG3  | 1:639:A:MET:HE1  | 6        | 0.49          |
| (1,3)   | 1:639:A:MET:HG3  | 1:639:A:MET:HE2  | 9        | 0.49          |
| (1,2)   | 1:639:A:MET:HG2  | 1:639:A:MET:HE3  | 16       | 0.49          |
| (1,2)   | 1:639:A:MET:HG2  | 1:639:A:MET:HE1  | 19       | 0.49          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD11 | 2        | 0.48          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD12 | 2        | 0.48          |
| (3,24)  | 1:628:A:LEU:HD21 | 2:545:B:LEU:HD13 | 2        | 0.48          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD11 | 2        | 0.48          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD12 | 2        | 0.48          |
| (3,24)  | 1:628:A:LEU:HD22 | 2:545:B:LEU:HD13 | 2        | 0.48          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD11 | 2        | 0.48          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD12 | 2        | 0.48          |
| (3,24)  | 1:628:A:LEU:HD23 | 2:545:B:LEU:HD13 | 2        | 0.48          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 11       | 0.48          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 11       | 0.48          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 11       | 0.48          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 11       | 0.48          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 11       | 0.48          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 11       | 0.48          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 11       | 0.48          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 11       | 0.48          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 11       | 0.48          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 16       | 0.48          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 16       | 0.48          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 16       | 0.48          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 16       | 0.48          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 16       | 0.48          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 16       | 0.48          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 11       | 0.48          |
| (2,267) | 2:542:B:PHE:H    | 2:540:B:MET:HB2  | 3        | 0.48          |
| (2,267) | 2:542:B:PHE:H    | 2:540:B:MET:HB2  | 14       | 0.48          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG22 | 15       | 0.48          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 12       | 0.48          |
| (2,190) | 2:543:B:SER:H    | 2:543:B:SER:HB2  | 7        | 0.48          |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 3        | 0.48          |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 8        | 0.48          |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD12 | 17       | 0.48          |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 6        | 0.48          |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 11       | 0.48          |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB2  | 15       | 0.48          |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB2  | 18       | 0.48          |
| (1,722) | 1:609:A:GLN:H    | 1:610:A:ALA:HB1  | 7        | 0.48          |
| (1,719) | 1:609:A:GLN:H    | 1:609:A:GLN:HG3  | 15       | 0.48          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 2        | 0.48          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 13       | 0.48          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 19       | 0.48          |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 13       | 0.48          |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 18       | 0.48          |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG23 | 12       | 0.48          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 13       | 0.48          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 17       | 0.48          |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD22 | 3        | 0.48          |
| (1,478) | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 17       | 0.48          |
| (1,457) | 1:608:A:VAL:HG21 | 1:605:A:HIS:HA   | 20       | 0.48          |
| (1,450) | 1:665:A:GLU:HA   | 1:665:A:GLU:HG2  | 7        | 0.48          |
| (1,424) | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 5        | 0.48          |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD22 | 10       | 0.48          |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD21 | 11       | 0.48          |
| (1,358) | 1:620:A:LEU:HD21 | 1:620:A:LEU:HB2  | 2        | 0.48          |
| (1,358) | 1:620:A:LEU:HD23 | 1:620:A:LEU:HB2  | 6        | 0.48          |
| (1,358) | 1:620:A:LEU:HD21 | 1:620:A:LEU:HB2  | 10       | 0.48          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG23 | 4        | 0.48          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG23 | 13       | 0.48          |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG22 | 14       | 0.48          |
| (1,225) | 1:632:A:ALA:HB2  | 1:604:A:VAL:HG21 | 1        | 0.48          |
| (1,225) | 1:632:A:ALA:HB3  | 1:604:A:VAL:HG21 | 7        | 0.48          |
| (1,96)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HD3  | 2        | 0.48          |
| (1,96)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HD3  | 9        | 0.48          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,96)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HD3  | 19       | 0.48          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 19       | 0.47          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 19       | 0.47          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 14       | 0.47          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 14       | 0.47          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 14       | 0.47          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 14       | 0.47          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 14       | 0.47          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 14       | 0.47          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 14       | 0.47          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 14       | 0.47          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 14       | 0.47          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 14       | 0.47          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG22 | 10       | 0.47          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG21 | 19       | 0.47          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 4        | 0.47          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 16       | 0.47          |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 4        | 0.47          |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 5        | 0.47          |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 14       | 0.47          |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 15       | 0.47          |
| (1,915) | 1:657:A:ILE:H    | 1:657:A:ILE:HD12 | 2        | 0.47          |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB1  | 1        | 0.47          |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB1  | 2        | 0.47          |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB2  | 6        | 0.47          |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 14       | 0.47          |
| (1,787) | 1:616:A:ASP:H    | 1:614:A:THR:HG21 | 14       | 0.47          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG23 | 10       | 0.47          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG21 | 20       | 0.47          |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 12       | 0.47          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG21 | 19       | 0.47          |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD12 | 16       | 0.47          |
| (1,548) | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 10       | 0.47          |
| (1,521) | 1:668:A:ARG:HD2  | 1:668:A:ARG:HG3  | 11       | 0.47          |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD22 | 11       | 0.47          |
| (1,483) | 1:667:A:LYS:HA   | 1:667:A:LYS:HG3  | 9        | 0.47          |
| (1,483) | 1:667:A:LYS:HA   | 1:667:A:LYS:HG3  | 14       | 0.47          |
| (1,480) | 1:653:A:LEU:HD21 | 1:636:A:GLU:HA   | 14       | 0.47          |
| (1,478) | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 18       | 0.47          |
| (1,470) | 1:635:A:VAL:HG12 | 1:639:A:MET:HE3  | 11       | 0.47          |
| (1,457) | 1:608:A:VAL:HG22 | 1:605:A:HIS:HA   | 9        | 0.47          |
| (1,359) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD23 | 9        | 0.47          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,358) | 1:620:A:LEU:HD23 | 1:620:A:LEU:HB2  | 1        | 0.47          |
| (1,358) | 1:620:A:LEU:HD23 | 1:620:A:LEU:HB2  | 19       | 0.47          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB2  | 2        | 0.47          |
| (1,302) | 1:614:A:THR:HG23 | 1:617:A:PRO:HA   | 19       | 0.47          |
| (1,84)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HG2  | 11       | 0.47          |
| (1,36)  | 1:609:A:GLN:HA   | 1:609:A:GLN:HG3  | 9        | 0.47          |
| (1,30)  | 1:649:A:TYR:HB3  | 1:643:A:ALA:HB3  | 12       | 0.47          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 12       | 0.46          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 12       | 0.46          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 12       | 0.46          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 12       | 0.46          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 12       | 0.46          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 12       | 0.46          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 12       | 0.46          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 12       | 0.46          |
| (3,8)   | 1:612:A:PHE:HE1  | 2:546:B:LEU:HA   | 20       | 0.46          |
| (3,8)   | 1:612:A:PHE:HE2  | 2:546:B:LEU:HA   | 20       | 0.46          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG22 | 14       | 0.46          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 11       | 0.46          |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 7        | 0.46          |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 13       | 0.46          |
| (1,986) | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 14       | 0.46          |
| (1,986) | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 17       | 0.46          |
| (1,951) | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 10       | 0.46          |
| (1,942) | 1:664:A:LEU:H    | 1:664:A:LEU:HD12 | 4        | 0.46          |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB1  | 5        | 0.46          |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB1  | 7        | 0.46          |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB3  | 16       | 0.46          |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB3  | 19       | 0.46          |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 6        | 0.46          |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 15       | 0.46          |
| (1,711) | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 15       | 0.46          |
| (1,701) | 1:614:A:THR:H    | 1:614:A:THR:HG21 | 8        | 0.46          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 3        | 0.46          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 15       | 0.46          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 18       | 0.46          |
| (1,603) | 1:599:A:LEU:HD12 | 1:595:A:VAL:HG13 | 5        | 0.46          |
| (1,485) | 1:635:A:VAL:HA   | 1:638:A:ASP:HB3  | 6        | 0.46          |
| (1,483) | 1:667:A:LYS:HA   | 1:667:A:LYS:HG3  | 1        | 0.46          |
| (1,483) | 1:667:A:LYS:HA   | 1:667:A:LYS:HG3  | 10       | 0.46          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 12       | 0.46          |
| (1,427) | 1:643:A:ALA:HB1  | 1:649:A:TYR:HD1  | 9        | 0.46          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,427) | 1:643:A:ALA:HB1  | 1:649:A:TYR:HD2  | 9        | 0.46          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG12 | 3        | 0.46          |
| (1,355) | 1:593:A:GLU:HA   | 1:593:A:GLU:HG2  | 1        | 0.46          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB3  | 4        | 0.46          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB3  | 19       | 0.46          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB3  | 20       | 0.46          |
| (1,284) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HA   | 14       | 0.46          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG21 | 3        | 0.46          |
| (1,225) | 1:632:A:ALA:HB3  | 1:604:A:VAL:HG22 | 13       | 0.46          |
| (1,225) | 1:632:A:ALA:HB3  | 1:604:A:VAL:HG21 | 16       | 0.46          |
| (1,221) | 1:607:A:LEU:HB3  | 1:604:A:VAL:HA   | 10       | 0.46          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB1  | 10       | 0.46          |
| (1,172) | 1:651:A:HIS:HB2  | 1:651:A:HIS:HD2  | 20       | 0.46          |
| (1,117) | 1:653:A:LEU:HD22 | 1:650:A:TYR:HD1  | 20       | 0.46          |
| (1,117) | 1:653:A:LEU:HD22 | 1:650:A:TYR:HD2  | 20       | 0.46          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 2        | 0.46          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 11       | 0.46          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 14       | 0.46          |
| (1,38)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HG2  | 10       | 0.46          |
| (1,38)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HG2  | 11       | 0.46          |
| (1,38)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HG2  | 14       | 0.46          |
| (1,36)  | 1:609:A:GLN:HA   | 1:609:A:GLN:HG3  | 3        | 0.46          |
| (1,36)  | 1:609:A:GLN:HA   | 1:609:A:GLN:HG3  | 16       | 0.46          |
| (1,36)  | 1:609:A:GLN:HA   | 1:609:A:GLN:HG3  | 19       | 0.46          |
| (1,36)  | 1:609:A:GLN:HA   | 1:609:A:GLN:HG3  | 20       | 0.46          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG21 | 2        | 0.45          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG22 | 2        | 0.45          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG23 | 2        | 0.45          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG21 | 2        | 0.45          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG22 | 2        | 0.45          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG23 | 2        | 0.45          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 10       | 0.45          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 10       | 0.45          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD21 | 10       | 0.45          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD22 | 10       | 0.45          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD23 | 10       | 0.45          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD21 | 10       | 0.45          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD22 | 10       | 0.45          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD23 | 10       | 0.45          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 5        | 0.45          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 5        | 0.45          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 5        | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,3)    | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 5        | 0.45          |
| (3,3)    | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 5        | 0.45          |
| (3,3)    | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 5        | 0.45          |
| (2,246)  | 2:537:B:ILE:H    | 2:537:B:ILE:HG21 | 5        | 0.45          |
| (2,246)  | 2:537:B:ILE:H    | 2:537:B:ILE:HG23 | 12       | 0.45          |
| (2,202)  | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 7        | 0.45          |
| (2,133)  | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 9        | 0.45          |
| (2,109)  | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 9        | 0.45          |
| (2,72)   | 2:537:B:ILE:HB   | 2:534:B:PHE:HD1  | 11       | 0.45          |
| (2,72)   | 2:537:B:ILE:HB   | 2:534:B:PHE:HD2  | 11       | 0.45          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD1  | 5        | 0.45          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD2  | 5        | 0.45          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD1  | 5        | 0.45          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD2  | 5        | 0.45          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD1  | 5        | 0.45          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD2  | 5        | 0.45          |
| (1,945)  | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 6        | 0.45          |
| (1,942)  | 1:664:A:LEU:H    | 1:664:A:LEU:HD12 | 8        | 0.45          |
| (1,942)  | 1:664:A:LEU:H    | 1:664:A:LEU:HD11 | 14       | 0.45          |
| (1,824)  | 1:628:A:LEU:H    | 1:630:A:ALA:HB3  | 8        | 0.45          |
| (1,824)  | 1:628:A:LEU:H    | 1:630:A:ALA:HB3  | 17       | 0.45          |
| (1,813)  | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 4        | 0.45          |
| (1,783)  | 1:616:A:ASP:H    | 1:615:A:PRO:HD3  | 7        | 0.45          |
| (1,711)  | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 9        | 0.45          |
| (1,710)  | 1:588:A:ARG:H    | 1:587:A:VAL:HG22 | 1        | 0.45          |
| (1,710)  | 1:588:A:ARG:H    | 1:587:A:VAL:HG23 | 10       | 0.45          |
| (1,657)  | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE1  | 1        | 0.45          |
| (1,657)  | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE2  | 1        | 0.45          |
| (1,639)  | 1:652:A:LEU:HD23 | 1:642:A:SER:HB2  | 3        | 0.45          |
| (1,606)  | 1:595:A:VAL:HA   | 1:599:A:LEU:HD23 | 5        | 0.45          |
| (1,495)  | 1:653:A:LEU:HD13 | 1:603:A:LEU:HD13 | 8        | 0.45          |
| (1,483)  | 1:667:A:LYS:HA   | 1:667:A:LYS:HG3  | 3        | 0.45          |
| (1,457)  | 1:608:A:VAL:HG21 | 1:605:A:HIS:HA   | 13       | 0.45          |
| (1,447)  | 1:599:A:LEU:HB3  | 1:599:A:LEU:HD11 | 8        | 0.45          |
| (1,392)  | 1:635:A:VAL:HG22 | 1:632:A:ALA:HA   | 11       | 0.45          |
| (1,371)  | 1:653:A:LEU:HB3  | 1:653:A:LEU:HD22 | 14       | 0.45          |
| (1,349)  | 1:610:A:ALA:HB1  | 1:657:A:ILE:HD12 | 6        | 0.45          |
| (1,247)  | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 3        | 0.45          |
| (1,247)  | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 6        | 0.45          |
| (1,247)  | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 8        | 0.45          |
| (1,247)  | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 9        | 0.45          |
| (1,247)  | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 10       | 0.45          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,247) | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 13       | 0.45          |
| (1,247) | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 16       | 0.45          |
| (1,247) | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 18       | 0.45          |
| (1,221) | 1:607:A:LEU:HB3  | 1:604:A:VAL:HA   | 5        | 0.45          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB1  | 1        | 0.45          |
| (1,172) | 1:651:A:HIS:HB2  | 1:651:A:HIS:HD2  | 6        | 0.45          |
| (1,172) | 1:651:A:HIS:HB2  | 1:651:A:HIS:HD2  | 7        | 0.45          |
| (1,172) | 1:651:A:HIS:HB2  | 1:651:A:HIS:HD2  | 16       | 0.45          |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 14       | 0.45          |
| (1,38)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HG2  | 2        | 0.45          |
| (1,38)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HG2  | 8        | 0.45          |
| (1,38)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HG2  | 12       | 0.45          |
| (1,38)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HG2  | 13       | 0.45          |
| (1,38)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HG2  | 17       | 0.45          |
| (1,36)  | 1:609:A:GLN:HA   | 1:609:A:GLN:HG3  | 1        | 0.45          |
| (1,36)  | 1:609:A:GLN:HA   | 1:609:A:GLN:HG3  | 18       | 0.45          |
| (2,252) | 2:535:B:SER:H    | 2:534:B:PHE:HD1  | 19       | 0.44          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 12       | 0.44          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 13       | 0.44          |
| (2,133) | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 19       | 0.44          |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 17       | 0.44          |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 18       | 0.44          |
| (1,951) | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 5        | 0.44          |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 19       | 0.44          |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD13 | 7        | 0.44          |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD11 | 20       | 0.44          |
| (1,921) | 1:659:A:LYS:H    | 1:659:A:LYS:HG3  | 4        | 0.44          |
| (1,921) | 1:659:A:LYS:H    | 1:659:A:LYS:HG3  | 8        | 0.44          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD1  | 10       | 0.44          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD2  | 10       | 0.44          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD1  | 14       | 0.44          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD2  | 14       | 0.44          |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB1  | 3        | 0.44          |
| (1,824) | 1:628:A:LEU:H    | 1:630:A:ALA:HB2  | 20       | 0.44          |
| (1,813) | 1:625:A:MET:H    | 1:625:A:MET:HG3  | 11       | 0.44          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG21 | 8        | 0.44          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG23 | 13       | 0.44          |
| (1,725) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HG3  | 17       | 0.44          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG23 | 15       | 0.44          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD13 | 3        | 0.44          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD11 | 10       | 0.44          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD12 | 11       | 0.44          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD12 | 13       | 0.44          |
| (1,583) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD11 | 14       | 0.44          |
| (1,548) | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 6        | 0.44          |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 15       | 0.44          |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 17       | 0.44          |
| (1,457) | 1:608:A:VAL:HG23 | 1:605:A:HIS:HA   | 3        | 0.44          |
| (1,447) | 1:599:A:LEU:HB3  | 1:599:A:LEU:HD13 | 11       | 0.44          |
| (1,447) | 1:599:A:LEU:HB3  | 1:599:A:LEU:HD12 | 15       | 0.44          |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG11 | 12       | 0.44          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG21 | 6        | 0.44          |
| (1,357) | 1:608:A:VAL:HG21 | 1:629:A:VAL:HA   | 8        | 0.44          |
| (1,357) | 1:608:A:VAL:HG21 | 1:629:A:VAL:HA   | 16       | 0.44          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB3  | 5        | 0.44          |
| (1,349) | 1:610:A:ALA:HB2  | 1:657:A:ILE:HD11 | 12       | 0.44          |
| (1,302) | 1:614:A:THR:HG22 | 1:617:A:PRO:HA   | 5        | 0.44          |
| (1,302) | 1:614:A:THR:HG22 | 1:617:A:PRO:HA   | 17       | 0.44          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 8        | 0.44          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 9        | 0.44          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 12       | 0.44          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 13       | 0.44          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 15       | 0.44          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 19       | 0.44          |
| (1,247) | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 5        | 0.44          |
| (1,247) | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 7        | 0.44          |
| (1,247) | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 11       | 0.44          |
| (1,247) | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 14       | 0.44          |
| (1,247) | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 19       | 0.44          |
| (1,223) | 1:604:A:VAL:HG11 | 1:604:A:VAL:HA   | 18       | 0.44          |
| (1,221) | 1:607:A:LEU:HB3  | 1:604:A:VAL:HA   | 18       | 0.44          |
| (1,209) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD23 | 7        | 0.44          |
| (1,172) | 1:651:A:HIS:HB2  | 1:651:A:HIS:HD2  | 15       | 0.44          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 17       | 0.44          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 18       | 0.44          |
| (1,85)  | 1:662:A:LYS:HA   | 1:662:A:LYS:HB2  | 20       | 0.44          |
| (1,36)  | 1:609:A:GLN:HA   | 1:609:A:GLN:HG3  | 4        | 0.44          |
| (1,36)  | 1:609:A:GLN:HA   | 1:609:A:GLN:HG3  | 6        | 0.44          |
| (1,2)   | 1:639:A:MET:HG2  | 1:639:A:MET:HE2  | 12       | 0.44          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 10       | 0.43          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 10       | 0.43          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 10       | 0.43          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 10       | 0.43          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 10       | 0.43          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 10       | 0.43          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG23 | 3        | 0.43          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG22 | 4        | 0.43          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG23 | 7        | 0.43          |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 2        | 0.43          |
| (2,77)  | 2:547:B:SER:HB3  | 2:544:B:ALA:HA   | 2        | 0.43          |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD11 | 1        | 0.43          |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD13 | 3        | 0.43          |
| (1,921) | 1:659:A:LYS:H    | 1:659:A:LYS:HG3  | 15       | 0.43          |
| (1,879) | 1:648:A:GLU:H    | 1:649:A:TYR:HB2  | 19       | 0.43          |
| (1,778) | 1:611:A:ILE:H    | 1:611:A:ILE:HG12 | 12       | 0.43          |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG23 | 12       | 0.43          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG21 | 14       | 0.43          |
| (1,715) | 1:610:A:ALA:H    | 1:609:A:GLN:HG3  | 17       | 0.43          |
| (1,711) | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 11       | 0.43          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 12       | 0.43          |
| (1,680) | 1:642:A:SER:H    | 1:642:A:SER:HB2  | 1        | 0.43          |
| (1,680) | 1:642:A:SER:H    | 1:642:A:SER:HB2  | 2        | 0.43          |
| (1,680) | 1:642:A:SER:H    | 1:642:A:SER:HB2  | 10       | 0.43          |
| (1,680) | 1:642:A:SER:H    | 1:642:A:SER:HB2  | 20       | 0.43          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD13 | 4        | 0.43          |
| (1,630) | 1:628:A:LEU:HB3  | 1:628:A:LEU:HD13 | 7        | 0.43          |
| (1,603) | 1:599:A:LEU:HD11 | 1:595:A:VAL:HG11 | 9        | 0.43          |
| (1,601) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HD1  | 16       | 0.43          |
| (1,601) | 1:595:A:VAL:HG11 | 1:640:A:TYR:HD2  | 16       | 0.43          |
| (1,548) | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 17       | 0.43          |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 3        | 0.43          |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 7        | 0.43          |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 8        | 0.43          |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 11       | 0.43          |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 12       | 0.43          |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 14       | 0.43          |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 19       | 0.43          |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 20       | 0.43          |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD21 | 13       | 0.43          |
| (1,483) | 1:667:A:LYS:HA   | 1:667:A:LYS:HG3  | 8        | 0.43          |
| (1,483) | 1:667:A:LYS:HA   | 1:667:A:LYS:HG3  | 13       | 0.43          |
| (1,415) | 1:620:A:LEU:HD22 | 1:625:A:MET:HG2  | 7        | 0.43          |
| (1,357) | 1:608:A:VAL:HG21 | 1:629:A:VAL:HA   | 2        | 0.43          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB3  | 3        | 0.43          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 1        | 0.43          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 3        | 0.43          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 6        | 0.43          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 7        | 0.43          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 10       | 0.43          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 11       | 0.43          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 14       | 0.43          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 16       | 0.43          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 17       | 0.43          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 18       | 0.43          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 20       | 0.43          |
| (1,247) | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 4        | 0.43          |
| (1,247) | 1:659:A:LYS:HD2  | 1:659:A:LYS:HE2  | 20       | 0.43          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG22 | 1        | 0.43          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG23 | 10       | 0.43          |
| (1,214) | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD13 | 18       | 0.43          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 8        | 0.43          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 16       | 0.43          |
| (1,36)  | 1:609:A:GLN:HA   | 1:609:A:GLN:HG3  | 5        | 0.43          |
| (3,31)  | 1:664:A:LEU:HD11 | 2:542:B:PHE:HD1  | 13       | 0.42          |
| (3,31)  | 1:664:A:LEU:HD11 | 2:542:B:PHE:HD2  | 13       | 0.42          |
| (3,31)  | 1:664:A:LEU:HD12 | 2:542:B:PHE:HD1  | 13       | 0.42          |
| (3,31)  | 1:664:A:LEU:HD12 | 2:542:B:PHE:HD2  | 13       | 0.42          |
| (3,31)  | 1:664:A:LEU:HD13 | 2:542:B:PHE:HD1  | 13       | 0.42          |
| (3,31)  | 1:664:A:LEU:HD13 | 2:542:B:PHE:HD2  | 13       | 0.42          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 10       | 0.42          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 10       | 0.42          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 10       | 0.42          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 10       | 0.42          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 10       | 0.42          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 10       | 0.42          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 2        | 0.42          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 2        | 0.42          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 2        | 0.42          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 2        | 0.42          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 2        | 0.42          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 2        | 0.42          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 2        | 0.42          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 2        | 0.42          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 2        | 0.42          |
| (3,6)   | 1:612:A:PHE:HE1  | 2:545:B:LEU:HD21 | 12       | 0.42          |
| (3,6)   | 1:612:A:PHE:HE1  | 2:545:B:LEU:HD22 | 12       | 0.42          |
| (3,6)   | 1:612:A:PHE:HE1  | 2:545:B:LEU:HD23 | 12       | 0.42          |
| (3,6)   | 1:612:A:PHE:HE2  | 2:545:B:LEU:HD21 | 12       | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,6)    | 1:612:A:PHE:HE2  | 2:545:B:LEU:HD22 | 12       | 0.42          |
| (3,6)    | 1:612:A:PHE:HE2  | 2:545:B:LEU:HD23 | 12       | 0.42          |
| (2,246)  | 2:537:B:ILE:H    | 2:537:B:ILE:HG23 | 13       | 0.42          |
| (2,246)  | 2:537:B:ILE:H    | 2:537:B:ILE:HG23 | 17       | 0.42          |
| (2,202)  | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 3        | 0.42          |
| (2,200)  | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 18       | 0.42          |
| (2,133)  | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 6        | 0.42          |
| (2,132)  | 2:546:B:LEU:HB2  | 2:543:B:SER:HA   | 20       | 0.42          |
| (2,109)  | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 10       | 0.42          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 5        | 0.42          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 5        | 0.42          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 5        | 0.42          |
| (1,951)  | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 20       | 0.42          |
| (1,942)  | 1:664:A:LEU:H    | 1:664:A:LEU:HD11 | 10       | 0.42          |
| (1,937)  | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 19       | 0.42          |
| (1,931)  | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 12       | 0.42          |
| (1,925)  | 1:660:A:ILE:H    | 1:660:A:ILE:HD11 | 2        | 0.42          |
| (1,921)  | 1:659:A:LYS:H    | 1:659:A:LYS:HG3  | 5        | 0.42          |
| (1,921)  | 1:659:A:LYS:H    | 1:659:A:LYS:HG3  | 17       | 0.42          |
| (1,915)  | 1:657:A:ILE:H    | 1:657:A:ILE:HD13 | 17       | 0.42          |
| (1,843)  | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 5        | 0.42          |
| (1,843)  | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 15       | 0.42          |
| (1,787)  | 1:616:A:ASP:H    | 1:614:A:THR:HG21 | 11       | 0.42          |
| (1,743)  | 1:599:A:LEU:H    | 1:596:A:THR:HG22 | 3        | 0.42          |
| (1,743)  | 1:599:A:LEU:H    | 1:596:A:THR:HG22 | 18       | 0.42          |
| (1,682)  | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 7        | 0.42          |
| (1,682)  | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 10       | 0.42          |
| (1,682)  | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 14       | 0.42          |
| (1,680)  | 1:642:A:SER:H    | 1:642:A:SER:HB2  | 6        | 0.42          |
| (1,680)  | 1:642:A:SER:H    | 1:642:A:SER:HB2  | 18       | 0.42          |
| (1,670)  | 1:620:A:LEU:H    | 1:620:A:LEU:HD11 | 14       | 0.42          |
| (1,657)  | 1:595:A:VAL:HG12 | 1:649:A:TYR:HE1  | 4        | 0.42          |
| (1,657)  | 1:595:A:VAL:HG12 | 1:649:A:TYR:HE2  | 4        | 0.42          |
| (1,644)  | 1:608:A:VAL:HA   | 1:611:A:ILE:HD13 | 11       | 0.42          |
| (1,606)  | 1:595:A:VAL:HA   | 1:599:A:LEU:HD21 | 1        | 0.42          |
| (1,571)  | 1:591:A:TRP:HD1  | 1:589:A:LYS:HA   | 9        | 0.42          |
| (1,541)  | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 1        | 0.42          |
| (1,541)  | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 5        | 0.42          |
| (1,541)  | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 6        | 0.42          |
| (1,541)  | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 9        | 0.42          |
| (1,541)  | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 10       | 0.42          |
| (1,541)  | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 16       | 0.42          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 18       | 0.42          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 19       | 0.42          |
| (1,503) | 1:625:A:MET:HG2  | 1:629:A:VAL:HG21 | 9        | 0.42          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 10       | 0.42          |
| (1,447) | 1:599:A:LEU:HB3  | 1:599:A:LEU:HD12 | 3        | 0.42          |
| (1,447) | 1:599:A:LEU:HB3  | 1:599:A:LEU:HD13 | 19       | 0.42          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG21 | 10       | 0.42          |
| (1,357) | 1:608:A:VAL:HG22 | 1:629:A:VAL:HA   | 11       | 0.42          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB1  | 13       | 0.42          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB2  | 16       | 0.42          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 4        | 0.42          |
| (1,162) | 1:594:A:HIS:HB2  | 1:594:A:HIS:HD2  | 18       | 0.42          |
| (1,2)   | 1:639:A:MET:HG2  | 1:639:A:MET:HE2  | 4        | 0.42          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 4        | 0.41          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 4        | 0.41          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 13       | 0.41          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 13       | 0.41          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 9        | 0.41          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 9        | 0.41          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 9        | 0.41          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 9        | 0.41          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 9        | 0.41          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 9        | 0.41          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 19       | 0.41          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG21 | 6        | 0.41          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG23 | 16       | 0.41          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG21 | 18       | 0.41          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 3        | 0.41          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 7        | 0.41          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 8        | 0.41          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 14       | 0.41          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 15       | 0.41          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 19       | 0.41          |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 20       | 0.41          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 6        | 0.41          |
| (2,133) | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 2        | 0.41          |
| (2,133) | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 5        | 0.41          |
| (2,133) | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 15       | 0.41          |
| (2,132) | 2:546:B:LEU:HB2  | 2:543:B:SER:HA   | 18       | 0.41          |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 1        | 0.41          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 12       | 0.41          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 12       | 0.41          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 12       | 0.41          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 14       | 0.41          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 14       | 0.41          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 14       | 0.41          |
| (1,945) | 1:666:A:GLU:H    | 1:666:A:GLU:HG3  | 11       | 0.41          |
| (1,942) | 1:664:A:LEU:H    | 1:664:A:LEU:HD11 | 1        | 0.41          |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD12 | 8        | 0.41          |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD13 | 15       | 0.41          |
| (1,921) | 1:659:A:LYS:H    | 1:659:A:LYS:HG3  | 20       | 0.41          |
| (1,903) | 1:653:A:LEU:H    | 1:653:A:LEU:HD13 | 8        | 0.41          |
| (1,853) | 1:635:A:VAL:H    | 1:635:A:VAL:HG12 | 15       | 0.41          |
| (1,787) | 1:616:A:ASP:H    | 1:614:A:THR:HG21 | 6        | 0.41          |
| (1,783) | 1:616:A:ASP:H    | 1:615:A:PRO:HD3  | 14       | 0.41          |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG23 | 5        | 0.41          |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG23 | 7        | 0.41          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG21 | 17       | 0.41          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 4        | 0.41          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 5        | 0.41          |
| (1,680) | 1:642:A:SER:H    | 1:642:A:SER:HB2  | 3        | 0.41          |
| (1,680) | 1:642:A:SER:H    | 1:642:A:SER:HB2  | 9        | 0.41          |
| (1,680) | 1:642:A:SER:H    | 1:642:A:SER:HB2  | 11       | 0.41          |
| (1,680) | 1:642:A:SER:H    | 1:642:A:SER:HB2  | 17       | 0.41          |
| (1,680) | 1:642:A:SER:H    | 1:642:A:SER:HB2  | 19       | 0.41          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD12 | 9        | 0.41          |
| (1,640) | 1:639:A:MET:HB3  | 1:653:A:LEU:HD12 | 9        | 0.41          |
| (1,608) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HD22 | 9        | 0.41          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD1  | 13       | 0.41          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD2  | 13       | 0.41          |
| (1,572) | 1:654:A:ALA:HB2  | 1:657:A:ILE:HD11 | 9        | 0.41          |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 2        | 0.41          |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 4        | 0.41          |
| (1,541) | 1:606:A:LYS:HG2  | 1:606:A:LYS:HD2  | 13       | 0.41          |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD21 | 5        | 0.41          |
| (1,483) | 1:667:A:LYS:HA   | 1:667:A:LYS:HG3  | 6        | 0.41          |
| (1,483) | 1:667:A:LYS:HA   | 1:667:A:LYS:HG3  | 17       | 0.41          |
| (1,447) | 1:599:A:LEU:HB3  | 1:599:A:LEU:HD12 | 7        | 0.41          |
| (1,424) | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 13       | 0.41          |
| (1,411) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HB3  | 18       | 0.41          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 15       | 0.41          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG11 | 6        | 0.41          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG13 | 15       | 0.41          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG13 | 20       | 0.41          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,364) | 1:648:A:GLU:HA   | 1:651:A:HIS:HB2  | 20       | 0.41          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG21 | 5        | 0.41          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG21 | 14       | 0.41          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG23 | 17       | 0.41          |
| (1,357) | 1:608:A:VAL:HG23 | 1:629:A:VAL:HA   | 6        | 0.41          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB1  | 8        | 0.41          |
| (1,274) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB3  | 16       | 0.41          |
| (1,274) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB3  | 18       | 0.41          |
| (1,232) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG22 | 8        | 0.41          |
| (1,221) | 1:607:A:LEU:HB3  | 1:604:A:VAL:HA   | 1        | 0.41          |
| (1,209) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD22 | 3        | 0.41          |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 6        | 0.41          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 9        | 0.41          |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 16       | 0.41          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 8        | 0.41          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 7        | 0.41          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 15       | 0.41          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE1  | 1        | 0.4           |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE2  | 1        | 0.4           |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE1  | 1        | 0.4           |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE2  | 1        | 0.4           |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE1  | 1        | 0.4           |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE2  | 1        | 0.4           |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 1        | 0.4           |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 1        | 0.4           |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 1        | 0.4           |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 1        | 0.4           |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 1        | 0.4           |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 1        | 0.4           |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG21 | 8        | 0.4           |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 3        | 0.4           |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 13       | 0.4           |
| (2,214) | 2:534:B:PHE:H    | 2:533:B:ASP:HA   | 16       | 0.4           |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 7        | 0.4           |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 9        | 0.4           |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 10       | 0.4           |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 19       | 0.4           |
| (2,169) | 2:544:B:ALA:HA   | 2:547:B:SER:HB3  | 17       | 0.4           |
| (2,133) | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 14       | 0.4           |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 12       | 0.4           |
| (2,95)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HB3  | 3        | 0.4           |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 6        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,4)    | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 6        | 0.4           |
| (2,4)    | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 6        | 0.4           |
| (2,4)    | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 11       | 0.4           |
| (2,4)    | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 11       | 0.4           |
| (2,4)    | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 11       | 0.4           |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 19       | 0.4           |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 19       | 0.4           |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 19       | 0.4           |
| (1,942)  | 1:664:A:LEU:H    | 1:664:A:LEU:HD12 | 12       | 0.4           |
| (1,942)  | 1:664:A:LEU:H    | 1:664:A:LEU:HD12 | 13       | 0.4           |
| (1,937)  | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 3        | 0.4           |
| (1,931)  | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 18       | 0.4           |
| (1,925)  | 1:660:A:ILE:H    | 1:660:A:ILE:HD12 | 9        | 0.4           |
| (1,843)  | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 17       | 0.4           |
| (1,825)  | 1:634:A:LYS:H    | 1:634:A:LYS:HB2  | 14       | 0.4           |
| (1,804)  | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 11       | 0.4           |
| (1,804)  | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 17       | 0.4           |
| (1,762)  | 1:605:A:HIS:H    | 1:604:A:VAL:HG21 | 17       | 0.4           |
| (1,711)  | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 16       | 0.4           |
| (1,701)  | 1:614:A:THR:H    | 1:614:A:THR:HG21 | 9        | 0.4           |
| (1,680)  | 1:642:A:SER:H    | 1:642:A:SER:HB2  | 12       | 0.4           |
| (1,657)  | 1:595:A:VAL:HG12 | 1:649:A:TYR:HE1  | 18       | 0.4           |
| (1,657)  | 1:595:A:VAL:HG12 | 1:649:A:TYR:HE2  | 18       | 0.4           |
| (1,644)  | 1:608:A:VAL:HA   | 1:611:A:ILE:HD13 | 7        | 0.4           |
| (1,572)  | 1:654:A:ALA:HB2  | 1:657:A:ILE:HD11 | 19       | 0.4           |
| (1,478)  | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 9        | 0.4           |
| (1,457)  | 1:608:A:VAL:HG21 | 1:605:A:HIS:HA   | 10       | 0.4           |
| (1,447)  | 1:599:A:LEU:HB3  | 1:599:A:LEU:HD12 | 4        | 0.4           |
| (1,447)  | 1:599:A:LEU:HB3  | 1:599:A:LEU:HD12 | 12       | 0.4           |
| (1,424)  | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 2        | 0.4           |
| (1,394)  | 1:635:A:VAL:HG12 | 1:632:A:ALA:HA   | 10       | 0.4           |
| (1,392)  | 1:635:A:VAL:HG22 | 1:632:A:ALA:HA   | 9        | 0.4           |
| (1,373)  | 1:626:A:GLU:HA   | 1:629:A:VAL:HG12 | 8        | 0.4           |
| (1,363)  | 1:654:A:ALA:HA   | 1:657:A:ILE:HG22 | 13       | 0.4           |
| (1,357)  | 1:608:A:VAL:HG22 | 1:629:A:VAL:HA   | 5        | 0.4           |
| (1,357)  | 1:608:A:VAL:HG23 | 1:629:A:VAL:HA   | 14       | 0.4           |
| (1,357)  | 1:608:A:VAL:HG21 | 1:629:A:VAL:HA   | 18       | 0.4           |
| (1,357)  | 1:608:A:VAL:HG21 | 1:629:A:VAL:HA   | 19       | 0.4           |
| (1,352)  | 1:657:A:ILE:HB   | 1:654:A:ALA:HB3  | 9        | 0.4           |
| (1,352)  | 1:657:A:ILE:HB   | 1:654:A:ALA:HB3  | 10       | 0.4           |
| (1,352)  | 1:657:A:ILE:HB   | 1:654:A:ALA:HB2  | 11       | 0.4           |
| (1,352)  | 1:657:A:ILE:HB   | 1:654:A:ALA:HB2  | 17       | 0.4           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,301) | 1:620:A:LEU:HG   | 1:617:A:PRO:HA   | 15       | 0.4           |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG12 | 9        | 0.4           |
| (1,284) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HA   | 9        | 0.4           |
| (1,275) | 1:593:A:GLU:HB3  | 1:593:A:GLU:HG2  | 8        | 0.4           |
| (1,274) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB3  | 3        | 0.4           |
| (1,274) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB3  | 4        | 0.4           |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 5        | 0.4           |
| (1,225) | 1:632:A:ALA:HB2  | 1:604:A:VAL:HG22 | 4        | 0.4           |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 1        | 0.4           |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 5        | 0.4           |
| (1,186) | 1:621:A:LYS:HA   | 1:621:A:LYS:HG3  | 20       | 0.4           |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 6        | 0.4           |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 16       | 0.4           |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 12       | 0.4           |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 17       | 0.4           |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 19       | 0.4           |
| (1,2)   | 1:639:A:MET:HG2  | 1:639:A:MET:HE1  | 18       | 0.4           |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 9        | 0.39          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 9        | 0.39          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 9        | 0.39          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 9        | 0.39          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 9        | 0.39          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 9        | 0.39          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 17       | 0.39          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 17       | 0.39          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 17       | 0.39          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 17       | 0.39          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 17       | 0.39          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 17       | 0.39          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 12       | 0.39          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 17       | 0.39          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG22 | 1        | 0.39          |
| (2,246) | 2:537:B:ILE:H    | 2:537:B:ILE:HG21 | 9        | 0.39          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 15       | 0.39          |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 8        | 0.39          |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 11       | 0.39          |
| (2,133) | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 7        | 0.39          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 2        | 0.39          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 2        | 0.39          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 2        | 0.39          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 8        | 0.39          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 8        | 0.39          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 8        | 0.39          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 9        | 0.39          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 9        | 0.39          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 9        | 0.39          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 16       | 0.39          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 16       | 0.39          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 16       | 0.39          |
| (1,993) | 1:619:A:ALA:HB1  | 1:612:A:PHE:HZ   | 4        | 0.39          |
| (1,993) | 1:619:A:ALA:HB2  | 1:612:A:PHE:HZ   | 4        | 0.39          |
| (1,993) | 1:619:A:ALA:HB3  | 1:612:A:PHE:HZ   | 4        | 0.39          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 18       | 0.39          |
| (1,903) | 1:653:A:LEU:H    | 1:653:A:LEU:HD11 | 1        | 0.39          |
| (1,903) | 1:653:A:LEU:H    | 1:653:A:LEU:HD11 | 7        | 0.39          |
| (1,903) | 1:653:A:LEU:H    | 1:653:A:LEU:HD11 | 11       | 0.39          |
| (1,843) | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 1        | 0.39          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 2        | 0.39          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 20       | 0.39          |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG22 | 3        | 0.39          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG22 | 11       | 0.39          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG21 | 4        | 0.39          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG23 | 13       | 0.39          |
| (1,583) | 1:603:A:LEU:HD13 | 1:599:A:LEU:HD11 | 3        | 0.39          |
| (1,572) | 1:654:A:ALA:HB2  | 1:657:A:ILE:HD13 | 5        | 0.39          |
| (1,509) | 1:614:A:THR:HB   | 1:615:A:PRO:HD3  | 18       | 0.39          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 2        | 0.39          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 19       | 0.39          |
| (1,459) | 1:607:A:LEU:HB2  | 1:607:A:LEU:HD22 | 4        | 0.39          |
| (1,459) | 1:607:A:LEU:HB2  | 1:607:A:LEU:HD21 | 6        | 0.39          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 11       | 0.39          |
| (1,447) | 1:599:A:LEU:HB3  | 1:599:A:LEU:HD13 | 20       | 0.39          |
| (1,396) | 1:664:A:LEU:HD22 | 1:664:A:LEU:HB2  | 3        | 0.39          |
| (1,357) | 1:608:A:VAL:HG21 | 1:629:A:VAL:HA   | 3        | 0.39          |
| (1,357) | 1:608:A:VAL:HG22 | 1:629:A:VAL:HA   | 10       | 0.39          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB1  | 7        | 0.39          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB2  | 12       | 0.39          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG12 | 2        | 0.39          |
| (1,274) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB3  | 1        | 0.39          |
| (1,274) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB3  | 5        | 0.39          |
| (1,274) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB3  | 7        | 0.39          |
| (1,274) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB3  | 9        | 0.39          |
| (1,274) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB3  | 12       | 0.39          |
| (1,274) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB3  | 14       | 0.39          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG21 | 9        | 0.39          |
| (1,225) | 1:632:A:ALA:HB3  | 1:604:A:VAL:HG22 | 15       | 0.39          |
| (1,223) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HA   | 19       | 0.39          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 2        | 0.39          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 4        | 0.39          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 7        | 0.39          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 8        | 0.39          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 10       | 0.39          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 11       | 0.39          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 12       | 0.39          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 13       | 0.39          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 14       | 0.39          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 15       | 0.39          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 19       | 0.39          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 20       | 0.39          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 5        | 0.39          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 1        | 0.39          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 3        | 0.39          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 9        | 0.39          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 16       | 0.39          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 18       | 0.39          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 20       | 0.39          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD21 | 12       | 0.38          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD22 | 12       | 0.38          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD23 | 12       | 0.38          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD21 | 12       | 0.38          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD22 | 12       | 0.38          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD23 | 12       | 0.38          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 1        | 0.38          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 9        | 0.38          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 14       | 0.38          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 19       | 0.38          |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 1        | 0.38          |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 4        | 0.38          |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 14       | 0.38          |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 16       | 0.38          |
| (2,133) | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 11       | 0.38          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 19       | 0.38          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 19       | 0.38          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 19       | 0.38          |
| (2,93)  | 2:534:B:PHE:HD1  | 2:534:B:PHE:HB3  | 9        | 0.38          |
| (2,93)  | 2:534:B:PHE:HD2  | 2:534:B:PHE:HB3  | 9        | 0.38          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 3        | 0.38          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 3        | 0.38          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 17       | 0.38          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 17       | 0.38          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 17       | 0.38          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 19       | 0.38          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 19       | 0.38          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 19       | 0.38          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 20       | 0.38          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 20       | 0.38          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 20       | 0.38          |
| (1,986) | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 9        | 0.38          |
| (1,931) | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 9        | 0.38          |
| (1,931) | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 14       | 0.38          |
| (1,921) | 1:659:A:LYS:H    | 1:659:A:LYS:HG3  | 1        | 0.38          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 9        | 0.38          |
| (1,843) | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 9        | 0.38          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 4        | 0.38          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 8        | 0.38          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 10       | 0.38          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 14       | 0.38          |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG23 | 8        | 0.38          |
| (1,732) | 1:594:A:HIS:H    | 1:593:A:GLU:HB3  | 1        | 0.38          |
| (1,711) | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 19       | 0.38          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 1        | 0.38          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 8        | 0.38          |
| (1,665) | 1:592:A:HIS:H    | 1:592:A:HIS:HB2  | 9        | 0.38          |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG23 | 20       | 0.38          |
| (1,657) | 1:595:A:VAL:HG12 | 1:649:A:TYR:HE1  | 15       | 0.38          |
| (1,657) | 1:595:A:VAL:HG12 | 1:649:A:TYR:HE2  | 15       | 0.38          |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD12 | 15       | 0.38          |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD22 | 17       | 0.38          |
| (1,457) | 1:608:A:VAL:HG23 | 1:605:A:HIS:HA   | 18       | 0.38          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 2        | 0.38          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 3        | 0.38          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 3        | 0.38          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 11       | 0.38          |
| (1,424) | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 1        | 0.38          |
| (1,424) | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 18       | 0.38          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG21 | 18       | 0.38          |
| (1,402) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HA   | 2        | 0.38          |
| (1,392) | 1:635:A:VAL:HG21 | 1:632:A:ALA:HA   | 8        | 0.38          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 6        | 0.38          |
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 15       | 0.38          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG23 | 1        | 0.38          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG22 | 11       | 0.38          |
| (1,357) | 1:608:A:VAL:HG23 | 1:629:A:VAL:HA   | 9        | 0.38          |
| (1,349) | 1:610:A:ALA:HB2  | 1:657:A:ILE:HD13 | 11       | 0.38          |
| (1,284) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HA   | 8        | 0.38          |
| (1,225) | 1:632:A:ALA:HB1  | 1:604:A:VAL:HG22 | 17       | 0.38          |
| (1,214) | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD13 | 10       | 0.38          |
| (1,209) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD23 | 12       | 0.38          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 3        | 0.38          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 6        | 0.38          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 9        | 0.38          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 16       | 0.38          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 17       | 0.38          |
| (1,189) | 1:598:A:ASP:HB2  | 1:598:A:ASP:HA   | 18       | 0.38          |
| (1,163) | 1:591:A:TRP:HA   | 1:594:A:HIS:HD2  | 2        | 0.38          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 13       | 0.38          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 20       | 0.38          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 19       | 0.38          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 5        | 0.38          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 6        | 0.38          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 13       | 0.38          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 14       | 0.38          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD21 | 17       | 0.37          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD22 | 17       | 0.37          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD23 | 17       | 0.37          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD21 | 17       | 0.37          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD22 | 17       | 0.37          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD23 | 17       | 0.37          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD21 | 18       | 0.37          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD22 | 18       | 0.37          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD23 | 18       | 0.37          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD21 | 18       | 0.37          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD22 | 18       | 0.37          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD23 | 18       | 0.37          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 7        | 0.37          |
| (2,133) | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 17       | 0.37          |
| (2,109) | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 19       | 0.37          |
| (2,93)  | 2:534:B:PHE:HD1  | 2:534:B:PHE:HB3  | 15       | 0.37          |
| (2,93)  | 2:534:B:PHE:HD2  | 2:534:B:PHE:HB3  | 15       | 0.37          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 1        | 0.37          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 1        | 0.37          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 1        | 0.37          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 4        | 0.37          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 4        | 0.37          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 4        | 0.37          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 18       | 0.37          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 18       | 0.37          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 18       | 0.37          |
| (1,950) | 1:671:A:ARG:H    | 1:671:A:ARG:HB2  | 4        | 0.37          |
| (1,942) | 1:664:A:LEU:H    | 1:664:A:LEU:HD12 | 5        | 0.37          |
| (1,942) | 1:664:A:LEU:H    | 1:664:A:LEU:HD11 | 20       | 0.37          |
| (1,937) | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 5        | 0.37          |
| (1,931) | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 16       | 0.37          |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD13 | 5        | 0.37          |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD11 | 14       | 0.37          |
| (1,921) | 1:659:A:LYS:H    | 1:659:A:LYS:HG3  | 14       | 0.37          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 3        | 0.37          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 5        | 0.37          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 15       | 0.37          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD1  | 20       | 0.37          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD2  | 20       | 0.37          |
| (1,808) | 1:622:A:ASP:H    | 1:622:A:ASP:HB3  | 19       | 0.37          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 3        | 0.37          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 6        | 0.37          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 9        | 0.37          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 13       | 0.37          |
| (1,783) | 1:616:A:ASP:H    | 1:615:A:PRO:HD3  | 2        | 0.37          |
| (1,783) | 1:616:A:ASP:H    | 1:615:A:PRO:HD3  | 4        | 0.37          |
| (1,783) | 1:616:A:ASP:H    | 1:615:A:PRO:HD3  | 11       | 0.37          |
| (1,732) | 1:594:A:HIS:H    | 1:593:A:GLU:HB3  | 19       | 0.37          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 16       | 0.37          |
| (1,650) | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 7        | 0.37          |
| (1,639) | 1:652:A:LEU:HD21 | 1:642:A:SER:HB2  | 19       | 0.37          |
| (1,592) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HE2  | 10       | 0.37          |
| (1,572) | 1:654:A:ALA:HB2  | 1:657:A:ILE:HD11 | 1        | 0.37          |
| (1,572) | 1:654:A:ALA:HB3  | 1:657:A:ILE:HD12 | 8        | 0.37          |
| (1,571) | 1:591:A:TRP:HD1  | 1:589:A:LYS:HA   | 20       | 0.37          |
| (1,535) | 1:639:A:MET:HG3  | 1:653:A:LEU:HD21 | 14       | 0.37          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 18       | 0.37          |
| (1,492) | 1:653:A:LEU:HG   | 1:636:A:GLU:HA   | 6        | 0.37          |
| (1,483) | 1:667:A:LYS:HA   | 1:667:A:LYS:HG3  | 4        | 0.37          |
| (1,459) | 1:607:A:LEU:HB2  | 1:607:A:LEU:HD21 | 5        | 0.37          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 14       | 0.37          |
| (1,375) | 1:633:A:LYS:HD2  | 1:629:A:VAL:HG13 | 6        | 0.37          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG11 | 2        | 0.37          |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD23 | 8        | 0.37          |
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 1        | 0.37          |
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 2        | 0.37          |
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 3        | 0.37          |
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 4        | 0.37          |
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 5        | 0.37          |
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 7        | 0.37          |
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 10       | 0.37          |
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 16       | 0.37          |
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 18       | 0.37          |
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 19       | 0.37          |
| (1,365) | 1:655:A:GLU:HB3  | 1:655:A:GLU:HA   | 20       | 0.37          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG22 | 7        | 0.37          |
| (1,357) | 1:608:A:VAL:HG21 | 1:629:A:VAL:HA   | 4        | 0.37          |
| (1,357) | 1:608:A:VAL:HG21 | 1:629:A:VAL:HA   | 12       | 0.37          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG22 | 8        | 0.37          |
| (1,231) | 1:601:A:SER:HA   | 1:604:A:VAL:HG23 | 17       | 0.37          |
| (1,223) | 1:604:A:VAL:HG11 | 1:604:A:VAL:HA   | 17       | 0.37          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 15       | 0.37          |
| (1,186) | 1:621:A:LYS:HA   | 1:621:A:LYS:HG3  | 10       | 0.37          |
| (1,142) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HE1  | 4        | 0.37          |
| (1,142) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HE2  | 4        | 0.37          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 4        | 0.37          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 15       | 0.37          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 9        | 0.37          |
| (3,34)  | 1:664:A:LEU:HD21 | 2:542:B:PHE:HE1  | 7        | 0.36          |
| (3,34)  | 1:664:A:LEU:HD21 | 2:542:B:PHE:HE2  | 7        | 0.36          |
| (3,34)  | 1:664:A:LEU:HD22 | 2:542:B:PHE:HE1  | 7        | 0.36          |
| (3,34)  | 1:664:A:LEU:HD22 | 2:542:B:PHE:HE2  | 7        | 0.36          |
| (3,34)  | 1:664:A:LEU:HD23 | 2:542:B:PHE:HE1  | 7        | 0.36          |
| (3,34)  | 1:664:A:LEU:HD23 | 2:542:B:PHE:HE2  | 7        | 0.36          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG21 | 20       | 0.36          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG22 | 20       | 0.36          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG23 | 20       | 0.36          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG21 | 20       | 0.36          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG22 | 20       | 0.36          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG23 | 20       | 0.36          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 15       | 0.36          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 15       | 0.36          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 8        | 0.36          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 1        | 0.36          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 10       | 0.36          |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 12       | 0.36          |
| (2,133) | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 1        | 0.36          |
| (2,133) | 2:546:B:LEU:HB3  | 2:543:B:SER:HA   | 8        | 0.36          |
| (2,93)  | 2:534:B:PHE:HD1  | 2:534:B:PHE:HB3  | 4        | 0.36          |
| (2,93)  | 2:534:B:PHE:HD2  | 2:534:B:PHE:HB3  | 4        | 0.36          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 5        | 0.36          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 5        | 0.36          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 5        | 0.36          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 10       | 0.36          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 10       | 0.36          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 10       | 0.36          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 15       | 0.36          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 15       | 0.36          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 15       | 0.36          |
| (1,942) | 1:664:A:LEU:H    | 1:664:A:LEU:HD12 | 9        | 0.36          |
| (1,931) | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 5        | 0.36          |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD13 | 4        | 0.36          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 10       | 0.36          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 1        | 0.36          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 16       | 0.36          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 18       | 0.36          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 19       | 0.36          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG22 | 6        | 0.36          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG22 | 2        | 0.36          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 9        | 0.36          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD11 | 16       | 0.36          |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG22 | 17       | 0.36          |
| (1,650) | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 16       | 0.36          |
| (1,629) | 1:625:A:MET:HA   | 1:628:A:LEU:HD23 | 3        | 0.36          |
| (1,590) | 1:599:A:LEU:HG   | 1:599:A:LEU:HB3  | 1        | 0.36          |
| (1,590) | 1:599:A:LEU:HG   | 1:599:A:LEU:HB3  | 5        | 0.36          |
| (1,590) | 1:599:A:LEU:HG   | 1:599:A:LEU:HB3  | 9        | 0.36          |
| (1,590) | 1:599:A:LEU:HG   | 1:599:A:LEU:HB3  | 17       | 0.36          |
| (1,590) | 1:599:A:LEU:HG   | 1:599:A:LEU:HB3  | 18       | 0.36          |
| (1,583) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD11 | 9        | 0.36          |
| (1,536) | 1:636:A:GLU:HG2  | 1:653:A:LEU:HD21 | 15       | 0.36          |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 14       | 0.36          |
| (1,446) | 1:658:A:TYR:HB2  | 1:655:A:GLU:HA   | 19       | 0.36          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG23 | 12       | 0.36          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,392) | 1:635:A:VAL:HG21 | 1:632:A:ALA:HA   | 16       | 0.36          |
| (1,392) | 1:635:A:VAL:HG22 | 1:632:A:ALA:HA   | 17       | 0.36          |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG11 | 8        | 0.36          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG12 | 12       | 0.36          |
| (1,349) | 1:610:A:ALA:HB3  | 1:657:A:ILE:HD13 | 14       | 0.36          |
| (1,269) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HG2  | 2        | 0.36          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 11       | 0.36          |
| (1,186) | 1:621:A:LYS:HA   | 1:621:A:LYS:HG3  | 11       | 0.36          |
| (1,186) | 1:621:A:LYS:HA   | 1:621:A:LYS:HG3  | 14       | 0.36          |
| (1,162) | 1:594:A:HIS:HB2  | 1:594:A:HIS:HD2  | 14       | 0.36          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 1        | 0.36          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 7        | 0.36          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 2        | 0.36          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 4        | 0.36          |
| (1,37)  | 1:609:A:GLN:HB2  | 1:609:A:GLN:HA   | 8        | 0.36          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 6        | 0.35          |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 6        | 0.35          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE1  | 14       | 0.35          |
| (3,28)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HE2  | 14       | 0.35          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE1  | 14       | 0.35          |
| (3,28)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HE2  | 14       | 0.35          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE1  | 14       | 0.35          |
| (3,28)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HE2  | 14       | 0.35          |
| (3,23)  | 1:628:A:LEU:HD21 | 2:538:B:ALA:HA   | 6        | 0.35          |
| (3,23)  | 1:628:A:LEU:HD22 | 2:538:B:ALA:HA   | 6        | 0.35          |
| (3,23)  | 1:628:A:LEU:HD23 | 2:538:B:ALA:HA   | 6        | 0.35          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 2        | 0.35          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 2        | 0.35          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG21 | 4        | 0.35          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG22 | 4        | 0.35          |
| (3,19)  | 1:628:A:LEU:HB2  | 2:537:B:ILE:HG23 | 4        | 0.35          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG21 | 4        | 0.35          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG22 | 4        | 0.35          |
| (3,19)  | 1:628:A:LEU:HB3  | 2:537:B:ILE:HG23 | 4        | 0.35          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 17       | 0.35          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 17       | 0.35          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 17       | 0.35          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 17       | 0.35          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 17       | 0.35          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 17       | 0.35          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 17       | 0.35          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 17       | 0.35          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 17       | 0.35          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 7        | 0.35          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 2        | 0.35          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 9        | 0.35          |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 18       | 0.35          |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 3        | 0.35          |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 17       | 0.35          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 11       | 0.35          |
| (2,93)  | 2:534:B:PHE:HD1  | 2:534:B:PHE:HB3  | 1        | 0.35          |
| (2,93)  | 2:534:B:PHE:HD2  | 2:534:B:PHE:HB3  | 1        | 0.35          |
| (2,93)  | 2:534:B:PHE:HD1  | 2:534:B:PHE:HB3  | 3        | 0.35          |
| (2,93)  | 2:534:B:PHE:HD2  | 2:534:B:PHE:HB3  | 3        | 0.35          |
| (2,63)  | 2:549:B:ILE:HA   | 2:549:B:ILE:HD11 | 20       | 0.35          |
| (2,63)  | 2:549:B:ILE:HA   | 2:549:B:ILE:HD12 | 20       | 0.35          |
| (2,63)  | 2:549:B:ILE:HA   | 2:549:B:ILE:HD13 | 20       | 0.35          |
| (2,37)  | 2:549:B:ILE:HD11 | 2:549:B:ILE:HA   | 20       | 0.35          |
| (2,37)  | 2:549:B:ILE:HD12 | 2:549:B:ILE:HA   | 20       | 0.35          |
| (2,37)  | 2:549:B:ILE:HD13 | 2:549:B:ILE:HA   | 20       | 0.35          |
| (2,4)   | 2:545:B:LEU:HD11 | 2:545:B:LEU:HA   | 3        | 0.35          |
| (2,4)   | 2:545:B:LEU:HD12 | 2:545:B:LEU:HA   | 3        | 0.35          |
| (2,4)   | 2:545:B:LEU:HD13 | 2:545:B:LEU:HA   | 3        | 0.35          |
| (2,1)   | 2:542:B:PHE:HA   | 2:545:B:LEU:HD11 | 13       | 0.35          |
| (2,1)   | 2:542:B:PHE:HA   | 2:545:B:LEU:HD12 | 13       | 0.35          |
| (2,1)   | 2:542:B:PHE:HA   | 2:545:B:LEU:HD13 | 13       | 0.35          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 13       | 0.35          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 13       | 0.35          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 13       | 0.35          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 17       | 0.35          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 17       | 0.35          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 17       | 0.35          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 13       | 0.35          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 13       | 0.35          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 13       | 0.35          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 17       | 0.35          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 17       | 0.35          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 17       | 0.35          |
| (1,942) | 1:664:A:LEU:H    | 1:664:A:LEU:HD13 | 16       | 0.35          |
| (1,931) | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 1        | 0.35          |
| (1,931) | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 2        | 0.35          |
| (1,931) | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 11       | 0.35          |
| (1,931) | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 17       | 0.35          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 2        | 0.35          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 4        | 0.35          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 8        | 0.35          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 12       | 0.35          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 17       | 0.35          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 20       | 0.35          |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 12       | 0.35          |
| (1,843) | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 18       | 0.35          |
| (1,808) | 1:622:A:ASP:H    | 1:622:A:ASP:HB3  | 5        | 0.35          |
| (1,804) | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 12       | 0.35          |
| (1,762) | 1:605:A:HIS:H    | 1:604:A:VAL:HG21 | 4        | 0.35          |
| (1,742) | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 18       | 0.35          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG21 | 16       | 0.35          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 4        | 0.35          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 6        | 0.35          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 10       | 0.35          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 11       | 0.35          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 12       | 0.35          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 14       | 0.35          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 15       | 0.35          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 16       | 0.35          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 17       | 0.35          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 18       | 0.35          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 19       | 0.35          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 20       | 0.35          |
| (1,673) | 1:593:A:GLU:H    | 1:593:A:GLU:HB3  | 10       | 0.35          |
| (1,657) | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE1  | 7        | 0.35          |
| (1,657) | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE2  | 7        | 0.35          |
| (1,650) | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 1        | 0.35          |
| (1,650) | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 11       | 0.35          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 15       | 0.35          |
| (1,503) | 1:625:A:MET:HG2  | 1:629:A:VAL:HG23 | 8        | 0.35          |
| (1,478) | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 13       | 0.35          |
| (1,447) | 1:599:A:LEU:HB3  | 1:599:A:LEU:HD13 | 6        | 0.35          |
| (1,402) | 1:629:A:VAL:HG12 | 1:630:A:ALA:HA   | 15       | 0.35          |
| (1,394) | 1:635:A:VAL:HG11 | 1:632:A:ALA:HA   | 5        | 0.35          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG11 | 16       | 0.35          |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD23 | 13       | 0.35          |
| (1,355) | 1:593:A:GLU:HA   | 1:593:A:GLU:HG2  | 18       | 0.35          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB3  | 1        | 0.35          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB1  | 6        | 0.35          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG13 | 14       | 0.35          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG11 | 15       | 0.35          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,274) | 1:641:A:GLU:HG2 | 1:641:A:GLU:HB3  | 10       | 0.35          |
| (1,242) | 1:668:A:ARG:HB2 | 1:665:A:GLU:HA   | 11       | 0.35          |
| (1,231) | 1:601:A:SER:HA  | 1:604:A:VAL:HG21 | 14       | 0.35          |
| (1,214) | 1:607:A:LEU:HB3 | 1:607:A:LEU:HD13 | 19       | 0.35          |
| (1,207) | 1:632:A:ALA:HA  | 1:607:A:LEU:HD12 | 15       | 0.35          |
| (1,2)   | 1:639:A:MET:HG2 | 1:639:A:MET:HE3  | 2        | 0.35          |
| (3,9)   | 1:619:A:ALA:HB1 | 2:545:B:LEU:HD21 | 1        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB1 | 2:545:B:LEU:HD22 | 1        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB1 | 2:545:B:LEU:HD23 | 1        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB2 | 2:545:B:LEU:HD21 | 1        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB2 | 2:545:B:LEU:HD22 | 1        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB2 | 2:545:B:LEU:HD23 | 1        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB3 | 2:545:B:LEU:HD21 | 1        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB3 | 2:545:B:LEU:HD22 | 1        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB3 | 2:545:B:LEU:HD23 | 1        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB1 | 2:545:B:LEU:HD21 | 8        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB1 | 2:545:B:LEU:HD22 | 8        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB1 | 2:545:B:LEU:HD23 | 8        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB2 | 2:545:B:LEU:HD21 | 8        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB2 | 2:545:B:LEU:HD22 | 8        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB2 | 2:545:B:LEU:HD23 | 8        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB3 | 2:545:B:LEU:HD21 | 8        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB3 | 2:545:B:LEU:HD22 | 8        | 0.34          |
| (3,9)   | 1:619:A:ALA:HB3 | 2:545:B:LEU:HD23 | 8        | 0.34          |
| (2,230) | 2:539:B:ASP:H   | 2:538:B:ALA:HA   | 5        | 0.34          |
| (2,202) | 2:537:B:ILE:H   | 2:536:B:SER:HA   | 20       | 0.34          |
| (2,93)  | 2:534:B:PHE:HD1 | 2:534:B:PHE:HB3  | 6        | 0.34          |
| (2,93)  | 2:534:B:PHE:HD2 | 2:534:B:PHE:HB3  | 6        | 0.34          |
| (2,93)  | 2:534:B:PHE:HD1 | 2:534:B:PHE:HB3  | 8        | 0.34          |
| (2,93)  | 2:534:B:PHE:HD2 | 2:534:B:PHE:HB3  | 8        | 0.34          |
| (2,93)  | 2:534:B:PHE:HD1 | 2:534:B:PHE:HB3  | 18       | 0.34          |
| (2,93)  | 2:534:B:PHE:HD2 | 2:534:B:PHE:HB3  | 18       | 0.34          |
| (2,68)  | 2:545:B:LEU:HA  | 2:545:B:LEU:HD21 | 7        | 0.34          |
| (2,68)  | 2:545:B:LEU:HA  | 2:545:B:LEU:HD22 | 7        | 0.34          |
| (2,68)  | 2:545:B:LEU:HA  | 2:545:B:LEU:HD23 | 7        | 0.34          |
| (1,989) | 1:631:A:TYR:HD1 | 1:628:A:LEU:HD21 | 3        | 0.34          |
| (1,989) | 1:631:A:TYR:HD1 | 1:628:A:LEU:HD22 | 3        | 0.34          |
| (1,989) | 1:631:A:TYR:HD1 | 1:628:A:LEU:HD23 | 3        | 0.34          |
| (1,989) | 1:631:A:TYR:HD2 | 1:628:A:LEU:HD21 | 3        | 0.34          |
| (1,989) | 1:631:A:TYR:HD2 | 1:628:A:LEU:HD22 | 3        | 0.34          |
| (1,989) | 1:631:A:TYR:HD2 | 1:628:A:LEU:HD23 | 3        | 0.34          |
| (1,950) | 1:671:A:ARG:H   | 1:671:A:ARG:HB2  | 1        | 0.34          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,950) | 1:671:A:ARG:H    | 1:671:A:ARG:HB2  | 11       | 0.34          |
| (1,942) | 1:664:A:LEU:H    | 1:664:A:LEU:HD11 | 7        | 0.34          |
| (1,937) | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 18       | 0.34          |
| (1,931) | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 7        | 0.34          |
| (1,931) | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 13       | 0.34          |
| (1,931) | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 15       | 0.34          |
| (1,925) | 1:660:A:ILE:H    | 1:660:A:ILE:HD12 | 16       | 0.34          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 1        | 0.34          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 11       | 0.34          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 13       | 0.34          |
| (1,916) | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 16       | 0.34          |
| (1,915) | 1:657:A:ILE:H    | 1:657:A:ILE:HD11 | 1        | 0.34          |
| (1,903) | 1:653:A:LEU:H    | 1:653:A:LEU:HD12 | 4        | 0.34          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD1  | 19       | 0.34          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD2  | 19       | 0.34          |
| (1,783) | 1:616:A:ASP:H    | 1:615:A:PRO:HD3  | 6        | 0.34          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 6        | 0.34          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG22 | 9        | 0.34          |
| (1,725) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HG3  | 10       | 0.34          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 1        | 0.34          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 2        | 0.34          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 3        | 0.34          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 7        | 0.34          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 8        | 0.34          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 9        | 0.34          |
| (1,684) | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 13       | 0.34          |
| (1,682) | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 17       | 0.34          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD12 | 17       | 0.34          |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG22 | 19       | 0.34          |
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD11 | 2        | 0.34          |
| (1,592) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HE2  | 11       | 0.34          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 12       | 0.34          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 17       | 0.34          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 20       | 0.34          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 16       | 0.34          |
| (1,424) | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 4        | 0.34          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG23 | 6        | 0.34          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG22 | 16       | 0.34          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG22 | 19       | 0.34          |
| (1,358) | 1:620:A:LEU:HD21 | 1:620:A:LEU:HB2  | 7        | 0.34          |
| (1,357) | 1:608:A:VAL:HG23 | 1:629:A:VAL:HA   | 15       | 0.34          |
| (1,225) | 1:632:A:ALA:HB1  | 1:604:A:VAL:HG21 | 20       | 0.34          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,204) | 1:620:A:LEU:HB3  | 1:620:A:LEU:HD22 | 7        | 0.34          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB1  | 4        | 0.34          |
| (1,162) | 1:594:A:HIS:HB2  | 1:594:A:HIS:HD2  | 12       | 0.34          |
| (1,148) | 1:635:A:VAL:HG11 | 1:631:A:TYR:HE1  | 5        | 0.34          |
| (1,148) | 1:635:A:VAL:HG11 | 1:631:A:TYR:HE2  | 5        | 0.34          |
| (1,118) | 1:653:A:LEU:HB3  | 1:650:A:TYR:HA   | 13       | 0.34          |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD1  | 1        | 0.34          |
| (1,116) | 1:653:A:LEU:HD11 | 1:650:A:TYR:HD2  | 1        | 0.34          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 3        | 0.34          |
| (1,71)  | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 10       | 0.34          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG21 | 10       | 0.33          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG22 | 10       | 0.33          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG23 | 10       | 0.33          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG21 | 10       | 0.33          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG22 | 10       | 0.33          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG23 | 10       | 0.33          |
| (3,21)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD1  | 9        | 0.33          |
| (3,21)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD2  | 9        | 0.33          |
| (3,21)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD1  | 9        | 0.33          |
| (3,21)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD2  | 9        | 0.33          |
| (3,21)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD1  | 9        | 0.33          |
| (3,21)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD2  | 9        | 0.33          |
| (3,12)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD11 | 7        | 0.33          |
| (3,12)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD12 | 7        | 0.33          |
| (3,12)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD13 | 7        | 0.33          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 10       | 0.33          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 10       | 0.33          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 10       | 0.33          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 10       | 0.33          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 10       | 0.33          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 10       | 0.33          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 10       | 0.33          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 10       | 0.33          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 10       | 0.33          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 8        | 0.33          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 8        | 0.33          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 8        | 0.33          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 8        | 0.33          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 8        | 0.33          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 8        | 0.33          |
| (2,252) | 2:535:B:SER:H    | 2:534:B:PHE:HD1  | 1        | 0.33          |
| (2,250) | 2:534:B:PHE:H    | 2:534:B:PHE:HD1  | 15       | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,202)  | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 5        | 0.33          |
| (2,202)  | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 8        | 0.33          |
| (2,127)  | 2:542:B:PHE:HA   | 2:545:B:LEU:HB3  | 17       | 0.33          |
| (2,109)  | 2:537:B:ILE:HA   | 2:537:B:ILE:HG12 | 11       | 0.33          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD1  | 13       | 0.33          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD2  | 13       | 0.33          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD1  | 13       | 0.33          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD2  | 13       | 0.33          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD1  | 13       | 0.33          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD2  | 13       | 0.33          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD1  | 17       | 0.33          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD2  | 17       | 0.33          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD1  | 17       | 0.33          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD2  | 17       | 0.33          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD1  | 17       | 0.33          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD2  | 17       | 0.33          |
| (1,952)  | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 6        | 0.33          |
| (1,950)  | 1:671:A:ARG:H    | 1:671:A:ARG:HB2  | 17       | 0.33          |
| (1,942)  | 1:664:A:LEU:H    | 1:664:A:LEU:HD12 | 19       | 0.33          |
| (1,937)  | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 8        | 0.33          |
| (1,937)  | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 9        | 0.33          |
| (1,937)  | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 15       | 0.33          |
| (1,925)  | 1:660:A:ILE:H    | 1:660:A:ILE:HD11 | 18       | 0.33          |
| (1,916)  | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 6        | 0.33          |
| (1,916)  | 1:658:A:TYR:H    | 1:658:A:TYR:HB3  | 7        | 0.33          |
| (1,903)  | 1:653:A:LEU:H    | 1:653:A:LEU:HD11 | 20       | 0.33          |
| (1,804)  | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 7        | 0.33          |
| (1,783)  | 1:616:A:ASP:H    | 1:615:A:PRO:HD3  | 12       | 0.33          |
| (1,684)  | 1:601:A:SER:H    | 1:601:A:SER:HB2  | 5        | 0.33          |
| (1,682)  | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 20       | 0.33          |
| (1,665)  | 1:592:A:HIS:H    | 1:592:A:HIS:HB2  | 17       | 0.33          |
| (1,658)  | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG22 | 13       | 0.33          |
| (1,657)  | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE1  | 17       | 0.33          |
| (1,657)  | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE2  | 17       | 0.33          |
| (1,642)  | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD13 | 20       | 0.33          |
| (1,590)  | 1:599:A:LEU:HG   | 1:599:A:LEU:HB3  | 10       | 0.33          |
| (1,590)  | 1:599:A:LEU:HG   | 1:599:A:LEU:HB3  | 14       | 0.33          |
| (1,590)  | 1:599:A:LEU:HG   | 1:599:A:LEU:HB3  | 16       | 0.33          |
| (1,572)  | 1:654:A:ALA:HB2  | 1:657:A:ILE:HD13 | 4        | 0.33          |
| (1,546)  | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 3        | 0.33          |
| (1,546)  | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 7        | 0.33          |
| (1,546)  | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 8        | 0.33          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 19       | 0.33          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 8        | 0.33          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 19       | 0.33          |
| (1,478) | 1:636:A:GLU:HG2  | 1:636:A:GLU:HA   | 19       | 0.33          |
| (1,457) | 1:608:A:VAL:HG21 | 1:605:A:HIS:HA   | 5        | 0.33          |
| (1,402) | 1:629:A:VAL:HG11 | 1:630:A:ALA:HA   | 3        | 0.33          |
| (1,402) | 1:629:A:VAL:HG11 | 1:630:A:ALA:HA   | 8        | 0.33          |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD21 | 19       | 0.33          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG22 | 9        | 0.33          |
| (1,354) | 1:660:A:ILE:HD12 | 1:657:A:ILE:HA   | 6        | 0.33          |
| (1,352) | 1:657:A:ILE:HB   | 1:654:A:ALA:HB1  | 18       | 0.33          |
| (1,349) | 1:610:A:ALA:HB2  | 1:657:A:ILE:HD13 | 16       | 0.33          |
| (1,274) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB3  | 8        | 0.33          |
| (1,223) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HA   | 3        | 0.33          |
| (1,219) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD22 | 17       | 0.33          |
| (1,210) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD22 | 13       | 0.33          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 7        | 0.33          |
| (1,156) | 1:602:A:HIS:HA   | 1:605:A:HIS:HB3  | 14       | 0.33          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 4        | 0.33          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 7        | 0.33          |
| (3,31)  | 1:664:A:LEU:HD11 | 2:542:B:PHE:HD1  | 7        | 0.32          |
| (3,31)  | 1:664:A:LEU:HD11 | 2:542:B:PHE:HD2  | 7        | 0.32          |
| (3,31)  | 1:664:A:LEU:HD12 | 2:542:B:PHE:HD1  | 7        | 0.32          |
| (3,31)  | 1:664:A:LEU:HD12 | 2:542:B:PHE:HD2  | 7        | 0.32          |
| (3,31)  | 1:664:A:LEU:HD13 | 2:542:B:PHE:HD1  | 7        | 0.32          |
| (3,31)  | 1:664:A:LEU:HD13 | 2:542:B:PHE:HD2  | 7        | 0.32          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 14       | 0.32          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 14       | 0.32          |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD21 | 19       | 0.32          |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD22 | 19       | 0.32          |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD23 | 19       | 0.32          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 18       | 0.32          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 18       | 0.32          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 18       | 0.32          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 18       | 0.32          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 18       | 0.32          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 18       | 0.32          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 18       | 0.32          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 18       | 0.32          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 18       | 0.32          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 6        | 0.32          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 6        | 0.32          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 6        | 0.32          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 6        | 0.32          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 6        | 0.32          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 6        | 0.32          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 2        | 0.32          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 15       | 0.32          |
| (2,200) | 2:539:B:ASP:H    | 2:539:B:ASP:HB3  | 5        | 0.32          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 4        | 0.32          |
| (2,93)  | 2:534:B:PHE:HD1  | 2:534:B:PHE:HB3  | 17       | 0.32          |
| (2,93)  | 2:534:B:PHE:HD2  | 2:534:B:PHE:HB3  | 17       | 0.32          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 18       | 0.32          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 18       | 0.32          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD1  | 20       | 0.32          |
| (2,73)  | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD2  | 20       | 0.32          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD1  | 20       | 0.32          |
| (2,73)  | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD2  | 20       | 0.32          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD1  | 20       | 0.32          |
| (2,73)  | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD2  | 20       | 0.32          |
| (2,68)  | 2:545:B:LEU:HA   | 2:545:B:LEU:HD21 | 13       | 0.32          |
| (2,68)  | 2:545:B:LEU:HA   | 2:545:B:LEU:HD22 | 13       | 0.32          |
| (2,68)  | 2:545:B:LEU:HA   | 2:545:B:LEU:HD23 | 13       | 0.32          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 4        | 0.32          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 4        | 0.32          |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 4        | 0.32          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 4        | 0.32          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 4        | 0.32          |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 4        | 0.32          |
| (1,952) | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 3        | 0.32          |
| (1,952) | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 8        | 0.32          |
| (1,937) | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 16       | 0.32          |
| (1,937) | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 17       | 0.32          |
| (1,931) | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 20       | 0.32          |
| (1,881) | 1:648:A:GLU:H    | 1:643:A:ALA:HB1  | 13       | 0.32          |
| (1,864) | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 16       | 0.32          |
| (1,846) | 1:633:A:LYS:H    | 1:633:A:LYS:HD2  | 3        | 0.32          |
| (1,843) | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 8        | 0.32          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 17       | 0.32          |
| (1,743) | 1:599:A:LEU:H    | 1:596:A:THR:HG22 | 15       | 0.32          |
| (1,723) | 1:609:A:GLN:H    | 1:608:A:VAL:HG12 | 20       | 0.32          |
| (1,711) | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 6        | 0.32          |
| (1,657) | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE1  | 11       | 0.32          |
| (1,657) | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE2  | 11       | 0.32          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,592) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HE2  | 7        | 0.32          |
| (1,590) | 1:599:A:LEU:HG   | 1:599:A:LEU:HB3  | 13       | 0.32          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 2        | 0.32          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 4        | 0.32          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 5        | 0.32          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 9        | 0.32          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 18       | 0.32          |
| (1,457) | 1:608:A:VAL:HG22 | 1:605:A:HIS:HA   | 6        | 0.32          |
| (1,447) | 1:599:A:LEU:HB3  | 1:599:A:LEU:HD12 | 2        | 0.32          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG11 | 11       | 0.32          |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD22 | 20       | 0.32          |
| (1,355) | 1:593:A:GLU:HA   | 1:593:A:GLU:HG2  | 19       | 0.32          |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 4        | 0.32          |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 12       | 0.32          |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 16       | 0.32          |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 18       | 0.32          |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 19       | 0.32          |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 20       | 0.32          |
| (1,223) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HA   | 15       | 0.32          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 3        | 0.32          |
| (1,186) | 1:621:A:LYS:HA   | 1:621:A:LYS:HG3  | 5        | 0.32          |
| (1,122) | 1:595:A:VAL:HG23 | 1:649:A:TYR:HE1  | 17       | 0.32          |
| (1,122) | 1:595:A:VAL:HG23 | 1:649:A:TYR:HE2  | 17       | 0.32          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 13       | 0.32          |
| (1,21)  | 1:664:A:LEU:HD22 | 1:664:A:LEU:HD13 | 4        | 0.32          |
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD11 | 18       | 0.32          |
| (1,21)  | 1:664:A:LEU:HD22 | 1:664:A:LEU:HD13 | 19       | 0.32          |
| (1,21)  | 1:664:A:LEU:HD22 | 1:664:A:LEU:HD13 | 20       | 0.32          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 11       | 0.31          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 11       | 0.31          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 11       | 0.31          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 11       | 0.31          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 11       | 0.31          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 11       | 0.31          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 5        | 0.31          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 14       | 0.31          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 15       | 0.31          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 12       | 0.31          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 12       | 0.31          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 12       | 0.31          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 14       | 0.31          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 14       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,146)  | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 14       | 0.31          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 12       | 0.31          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 12       | 0.31          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 12       | 0.31          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 17       | 0.31          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 17       | 0.31          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 17       | 0.31          |
| (2,127)  | 2:542:B:PHE:HA   | 2:545:B:LEU:HB3  | 8        | 0.31          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 10       | 0.31          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 10       | 0.31          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 10       | 0.31          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 13       | 0.31          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 13       | 0.31          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 14       | 0.31          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 14       | 0.31          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 16       | 0.31          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 16       | 0.31          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 20       | 0.31          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 20       | 0.31          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD1  | 9        | 0.31          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD2  | 9        | 0.31          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD1  | 9        | 0.31          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD2  | 9        | 0.31          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD1  | 9        | 0.31          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD2  | 9        | 0.31          |
| (1,966)  | 1:661:A:GLN:H    | 1:660:A:ILE:HG22 | 16       | 0.31          |
| (1,951)  | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 16       | 0.31          |
| (1,951)  | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 18       | 0.31          |
| (1,942)  | 1:664:A:LEU:H    | 1:664:A:LEU:HD12 | 6        | 0.31          |
| (1,937)  | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 2        | 0.31          |
| (1,937)  | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 10       | 0.31          |
| (1,937)  | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 13       | 0.31          |
| (1,936)  | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 12       | 0.31          |
| (1,931)  | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 4        | 0.31          |
| (1,931)  | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 6        | 0.31          |
| (1,931)  | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 8        | 0.31          |
| (1,915)  | 1:657:A:ILE:H    | 1:657:A:ILE:HD12 | 8        | 0.31          |
| (1,903)  | 1:653:A:LEU:H    | 1:653:A:LEU:HD13 | 13       | 0.31          |
| (1,762)  | 1:605:A:HIS:H    | 1:604:A:VAL:HG22 | 14       | 0.31          |
| (1,743)  | 1:599:A:LEU:H    | 1:596:A:THR:HG22 | 1        | 0.31          |
| (1,724)  | 1:591:A:TRP:HE1  | 1:589:A:LYS:HD2  | 4        | 0.31          |
| (1,717)  | 1:610:A:ALA:H    | 1:657:A:ILE:HD13 | 8        | 0.31          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,711) | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 5        | 0.31          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG22 | 9        | 0.31          |
| (1,677) | 1:643:A:ALA:H    | 1:642:A:SER:HB2  | 6        | 0.31          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD13 | 2        | 0.31          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD13 | 8        | 0.31          |
| (1,650) | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 10       | 0.31          |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD13 | 13       | 0.31          |
| (1,572) | 1:654:A:ALA:HB2  | 1:657:A:ILE:HD11 | 15       | 0.31          |
| (1,548) | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 11       | 0.31          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 6        | 0.31          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 10       | 0.31          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 11       | 0.31          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 13       | 0.31          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 14       | 0.31          |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 16       | 0.31          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 20       | 0.31          |
| (1,462) | 1:659:A:LYS:HG3  | 1:656:A:LYS:HA   | 18       | 0.31          |
| (1,443) | 1:625:A:MET:HG2  | 1:625:A:MET:HE1  | 7        | 0.31          |
| (1,424) | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 7        | 0.31          |
| (1,411) | 1:629:A:VAL:HG12 | 1:630:A:ALA:HB2  | 5        | 0.31          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG13 | 9        | 0.31          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG11 | 13       | 0.31          |
| (1,364) | 1:648:A:GLU:HA   | 1:651:A:HIS:HB2  | 6        | 0.31          |
| (1,349) | 1:610:A:ALA:HB2  | 1:657:A:ILE:HD13 | 15       | 0.31          |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 1        | 0.31          |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 4        | 0.31          |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 11       | 0.31          |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 12       | 0.31          |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 17       | 0.31          |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 2        | 0.31          |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 9        | 0.31          |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 10       | 0.31          |
| (1,274) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB3  | 6        | 0.31          |
| (1,243) | 1:659:A:LYS:HD3  | 1:659:A:LYS:HA   | 7        | 0.31          |
| (1,206) | 1:620:A:LEU:HB3  | 1:620:A:LEU:HD13 | 15       | 0.31          |
| (1,122) | 1:595:A:VAL:HG22 | 1:649:A:TYR:HE1  | 18       | 0.31          |
| (1,122) | 1:595:A:VAL:HG22 | 1:649:A:TYR:HE2  | 18       | 0.31          |
| (1,99)  | 1:661:A:GLN:HB3  | 1:658:A:TYR:HA   | 19       | 0.31          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 2        | 0.31          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 6        | 0.31          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 17       | 0.31          |
| (1,23)  | 1:653:A:LEU:HB3  | 1:653:A:LEU:HD11 | 15       | 0.31          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD11 | 12       | 0.31          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 4        | 0.3           |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 4        | 0.3           |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 4        | 0.3           |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 4        | 0.3           |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 4        | 0.3           |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 4        | 0.3           |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 3        | 0.3           |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 3        | 0.3           |
| (2,202) | 2:537:B:ILE:H    | 2:536:B:SER:HA   | 17       | 0.3           |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 17       | 0.3           |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 6        | 0.3           |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 6        | 0.3           |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 6        | 0.3           |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 11       | 0.3           |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 11       | 0.3           |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 11       | 0.3           |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 8        | 0.3           |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 8        | 0.3           |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 8        | 0.3           |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 6        | 0.3           |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 6        | 0.3           |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 8        | 0.3           |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 8        | 0.3           |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 9        | 0.3           |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 9        | 0.3           |
| (2,72)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HD1  | 4        | 0.3           |
| (2,72)  | 2:537:B:ILE:HB   | 2:534:B:PHE:HD2  | 4        | 0.3           |
| (2,43)  | 2:549:B:ILE:HG13 | 2:549:B:ILE:HG21 | 20       | 0.3           |
| (2,43)  | 2:549:B:ILE:HG13 | 2:549:B:ILE:HG22 | 20       | 0.3           |
| (2,43)  | 2:549:B:ILE:HG13 | 2:549:B:ILE:HG23 | 20       | 0.3           |
| (1,986) | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 3        | 0.3           |
| (1,986) | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 10       | 0.3           |
| (1,942) | 1:664:A:LEU:H    | 1:664:A:LEU:HD13 | 11       | 0.3           |
| (1,937) | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 1        | 0.3           |
| (1,937) | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 7        | 0.3           |
| (1,936) | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 7        | 0.3           |
| (1,936) | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 15       | 0.3           |
| (1,936) | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 19       | 0.3           |
| (1,864) | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 4        | 0.3           |
| (1,864) | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 5        | 0.3           |
| (1,864) | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 9        | 0.3           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,864) | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 11       | 0.3           |
| (1,778) | 1:611:A:ILE:H    | 1:611:A:ILE:HG12 | 10       | 0.3           |
| (1,723) | 1:609:A:GLN:H    | 1:608:A:VAL:HG11 | 9        | 0.3           |
| (1,711) | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 18       | 0.3           |
| (1,672) | 1:593:A:GLU:H    | 1:593:A:GLU:HG2  | 13       | 0.3           |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG23 | 16       | 0.3           |
| (1,572) | 1:654:A:ALA:HB2  | 1:657:A:ILE:HD13 | 10       | 0.3           |
| (1,546) | 1:606:A:LYS:HE2  | 1:606:A:LYS:HD2  | 1        | 0.3           |
| (1,479) | 1:639:A:MET:HB3  | 1:636:A:GLU:HA   | 9        | 0.3           |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 18       | 0.3           |
| (1,392) | 1:635:A:VAL:HG21 | 1:632:A:ALA:HA   | 2        | 0.3           |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD23 | 2        | 0.3           |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG21 | 3        | 0.3           |
| (1,357) | 1:608:A:VAL:HG22 | 1:629:A:VAL:HA   | 13       | 0.3           |
| (1,302) | 1:614:A:THR:HG21 | 1:617:A:PRO:HA   | 11       | 0.3           |
| (1,302) | 1:614:A:THR:HG21 | 1:617:A:PRO:HA   | 14       | 0.3           |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG12 | 5        | 0.3           |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG12 | 11       | 0.3           |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 2        | 0.3           |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 10       | 0.3           |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 13       | 0.3           |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 15       | 0.3           |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 18       | 0.3           |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 19       | 0.3           |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 20       | 0.3           |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 1        | 0.3           |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 3        | 0.3           |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 5        | 0.3           |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 6        | 0.3           |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 8        | 0.3           |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 14       | 0.3           |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 15       | 0.3           |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 13       | 0.3           |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 4        | 0.3           |
| (1,225) | 1:632:A:ALA:HB1  | 1:604:A:VAL:HG23 | 14       | 0.3           |
| (1,223) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HA   | 14       | 0.3           |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 6        | 0.3           |
| (1,94)  | 1:662:A:LYS:HD3  | 1:662:A:LYS:HE3  | 3        | 0.3           |
| (1,94)  | 1:662:A:LYS:HD3  | 1:662:A:LYS:HE3  | 8        | 0.3           |
| (1,94)  | 1:662:A:LYS:HD3  | 1:662:A:LYS:HE3  | 9        | 0.3           |
| (1,94)  | 1:662:A:LYS:HD3  | 1:662:A:LYS:HE3  | 13       | 0.3           |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 8        | 0.3           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 18       | 0.3           |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 19       | 0.3           |
| (1,21)  | 1:664:A:LEU:HD23 | 1:664:A:LEU:HD11 | 3        | 0.3           |
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD13 | 14       | 0.3           |
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD13 | 17       | 0.3           |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG21 | 14       | 0.29          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG22 | 14       | 0.29          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG23 | 14       | 0.29          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG21 | 14       | 0.29          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG22 | 14       | 0.29          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG23 | 14       | 0.29          |
| (2,267) | 2:542:B:PHE:H    | 2:540:B:MET:HB2  | 7        | 0.29          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 2        | 0.29          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 9        | 0.29          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 15       | 0.29          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 16       | 0.29          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 20       | 0.29          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 2        | 0.29          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 2        | 0.29          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 2        | 0.29          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 2        | 0.29          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 8        | 0.29          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 8        | 0.29          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 8        | 0.29          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 9        | 0.29          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 9        | 0.29          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 9        | 0.29          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 16       | 0.29          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 16       | 0.29          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 16       | 0.29          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 2        | 0.29          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 2        | 0.29          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 2        | 0.29          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 15       | 0.29          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 15       | 0.29          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 15       | 0.29          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 12       | 0.29          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 12       | 0.29          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 15       | 0.29          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 15       | 0.29          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 19       | 0.29          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 19       | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,73)   | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD1  | 3        | 0.29          |
| (2,73)   | 2:537:B:ILE:HG21 | 2:534:B:PHE:HD2  | 3        | 0.29          |
| (2,73)   | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD1  | 3        | 0.29          |
| (2,73)   | 2:537:B:ILE:HG22 | 2:534:B:PHE:HD2  | 3        | 0.29          |
| (2,73)   | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD1  | 3        | 0.29          |
| (2,73)   | 2:537:B:ILE:HG23 | 2:534:B:PHE:HD2  | 3        | 0.29          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 8        | 0.29          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 8        | 0.29          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 8        | 0.29          |
| (1,993)  | 1:619:A:ALA:HB1  | 1:612:A:PHE:HZ   | 5        | 0.29          |
| (1,993)  | 1:619:A:ALA:HB2  | 1:612:A:PHE:HZ   | 5        | 0.29          |
| (1,993)  | 1:619:A:ALA:HB3  | 1:612:A:PHE:HZ   | 5        | 0.29          |
| (1,993)  | 1:619:A:ALA:HB1  | 1:612:A:PHE:HZ   | 9        | 0.29          |
| (1,993)  | 1:619:A:ALA:HB2  | 1:612:A:PHE:HZ   | 9        | 0.29          |
| (1,993)  | 1:619:A:ALA:HB3  | 1:612:A:PHE:HZ   | 9        | 0.29          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 2        | 0.29          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 2        | 0.29          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 8        | 0.29          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 8        | 0.29          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 12       | 0.29          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 12       | 0.29          |
| (1,951)  | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 2        | 0.29          |
| (1,951)  | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 7        | 0.29          |
| (1,942)  | 1:664:A:LEU:H    | 1:664:A:LEU:HD12 | 18       | 0.29          |
| (1,936)  | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 1        | 0.29          |
| (1,936)  | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 3        | 0.29          |
| (1,936)  | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 10       | 0.29          |
| (1,936)  | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 11       | 0.29          |
| (1,936)  | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 17       | 0.29          |
| (1,936)  | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 18       | 0.29          |
| (1,936)  | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 20       | 0.29          |
| (1,915)  | 1:657:A:ILE:H    | 1:657:A:ILE:HD11 | 9        | 0.29          |
| (1,881)  | 1:648:A:GLU:H    | 1:643:A:ALA:HB2  | 15       | 0.29          |
| (1,864)  | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 18       | 0.29          |
| (1,864)  | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 19       | 0.29          |
| (1,864)  | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 20       | 0.29          |
| (1,804)  | 1:621:A:LYS:H    | 1:621:A:LYS:HB3  | 15       | 0.29          |
| (1,783)  | 1:616:A:ASP:H    | 1:615:A:PRO:HD3  | 3        | 0.29          |
| (1,743)  | 1:599:A:LEU:H    | 1:596:A:THR:HG23 | 5        | 0.29          |
| (1,742)  | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 17       | 0.29          |
| (1,723)  | 1:609:A:GLN:H    | 1:608:A:VAL:HG11 | 2        | 0.29          |
| (1,723)  | 1:609:A:GLN:H    | 1:608:A:VAL:HG11 | 13       | 0.29          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,711) | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 8        | 0.29          |
| (1,677) | 1:643:A:ALA:H    | 1:642:A:SER:HB2  | 10       | 0.29          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD12 | 19       | 0.29          |
| (1,571) | 1:591:A:TRP:HD1  | 1:589:A:LYS:HA   | 11       | 0.29          |
| (1,549) | 1:603:A:LEU:HD22 | 1:606:A:LYS:HD2  | 9        | 0.29          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 4        | 0.29          |
| (1,503) | 1:625:A:MET:HG2  | 1:629:A:VAL:HG21 | 15       | 0.29          |
| (1,475) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG13 | 4        | 0.29          |
| (1,450) | 1:665:A:GLU:HA   | 1:665:A:GLU:HG2  | 8        | 0.29          |
| (1,424) | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 3        | 0.29          |
| (1,424) | 1:626:A:GLU:HA   | 1:626:A:GLU:HG2  | 16       | 0.29          |
| (1,423) | 1:629:A:VAL:HG12 | 1:626:A:GLU:HG2  | 19       | 0.29          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG23 | 14       | 0.29          |
| (1,392) | 1:635:A:VAL:HG21 | 1:632:A:ALA:HA   | 7        | 0.29          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG11 | 7        | 0.29          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG22 | 4        | 0.29          |
| (1,302) | 1:614:A:THR:HG21 | 1:617:A:PRO:HA   | 6        | 0.29          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 11       | 0.29          |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 5        | 0.29          |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 6        | 0.29          |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 13       | 0.29          |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 17       | 0.29          |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG21 | 10       | 0.29          |
| (1,198) | 1:620:A:LEU:HG   | 1:620:A:LEU:HA   | 7        | 0.29          |
| (1,94)  | 1:662:A:LYS:HD3  | 1:662:A:LYS:HE3  | 4        | 0.29          |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 5        | 0.29          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 3        | 0.29          |
| (1,21)  | 1:664:A:LEU:HD22 | 1:664:A:LEU:HD11 | 15       | 0.29          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 5        | 0.28          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 5        | 0.28          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 1        | 0.28          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 9        | 0.28          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 10       | 0.28          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 14       | 0.28          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 15       | 0.28          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 18       | 0.28          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 19       | 0.28          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 20       | 0.28          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 19       | 0.28          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 8        | 0.28          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 12       | 0.28          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 2        | 0.28          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 7        | 0.28          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 9        | 0.28          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 17       | 0.28          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 17       | 0.28          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 17       | 0.28          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 19       | 0.28          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 19       | 0.28          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 19       | 0.28          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 20       | 0.28          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 20       | 0.28          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 20       | 0.28          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 1        | 0.28          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 1        | 0.28          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 1        | 0.28          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 7        | 0.28          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 7        | 0.28          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 7        | 0.28          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 9        | 0.28          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 9        | 0.28          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 9        | 0.28          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 14       | 0.28          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 14       | 0.28          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 14       | 0.28          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 5        | 0.28          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 5        | 0.28          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 11       | 0.28          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 11       | 0.28          |
| (1,986) | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 6        | 0.28          |
| (1,986) | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 16       | 0.28          |
| (1,966) | 1:661:A:GLN:H    | 1:660:A:ILE:HG22 | 20       | 0.28          |
| (1,936) | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 4        | 0.28          |
| (1,936) | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 5        | 0.28          |
| (1,936) | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 8        | 0.28          |
| (1,936) | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 14       | 0.28          |
| (1,881) | 1:648:A:GLU:H    | 1:643:A:ALA:HB3  | 9        | 0.28          |
| (1,866) | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 9        | 0.28          |
| (1,864) | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 13       | 0.28          |
| (1,864) | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 14       | 0.28          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD1  | 7        | 0.28          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD2  | 7        | 0.28          |
| (1,787) | 1:616:A:ASP:H    | 1:614:A:THR:HG22 | 4        | 0.28          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 4        | 0.28          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,672) | 1:593:A:GLU:H    | 1:593:A:GLU:HG2  | 10       | 0.28          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD11 | 6        | 0.28          |
| (1,601) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HD1  | 3        | 0.28          |
| (1,601) | 1:595:A:VAL:HG12 | 1:640:A:TYR:HD2  | 3        | 0.28          |
| (1,601) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD1  | 12       | 0.28          |
| (1,601) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HD2  | 12       | 0.28          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD1  | 5        | 0.28          |
| (1,597) | 1:635:A:VAL:HG12 | 1:631:A:TYR:HD2  | 5        | 0.28          |
| (1,583) | 1:603:A:LEU:HD13 | 1:599:A:LEU:HD12 | 6        | 0.28          |
| (1,582) | 1:599:A:LEU:HD21 | 1:599:A:LEU:HD13 | 9        | 0.28          |
| (1,572) | 1:654:A:ALA:HB1  | 1:657:A:ILE:HD11 | 11       | 0.28          |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 13       | 0.28          |
| (1,459) | 1:607:A:LEU:HB2  | 1:607:A:LEU:HD21 | 1        | 0.28          |
| (1,459) | 1:607:A:LEU:HB2  | 1:607:A:LEU:HD21 | 13       | 0.28          |
| (1,457) | 1:608:A:VAL:HG23 | 1:605:A:HIS:HA   | 4        | 0.28          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 9        | 0.28          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG21 | 11       | 0.28          |
| (1,415) | 1:620:A:LEU:HD22 | 1:625:A:MET:HG2  | 13       | 0.28          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG11 | 10       | 0.28          |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD23 | 3        | 0.28          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG22 | 20       | 0.28          |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 3        | 0.28          |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 7        | 0.28          |
| (1,282) | 1:671:A:ARG:HA   | 1:671:A:ARG:HB2  | 16       | 0.28          |
| (1,279) | 1:668:A:ARG:HA   | 1:668:A:ARG:HB2  | 7        | 0.28          |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 17       | 0.28          |
| (1,223) | 1:604:A:VAL:HG11 | 1:604:A:VAL:HA   | 10       | 0.28          |
| (1,221) | 1:607:A:LEU:HB3  | 1:604:A:VAL:HA   | 19       | 0.28          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD1  | 3        | 0.28          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD2  | 3        | 0.28          |
| (1,94)  | 1:662:A:LYS:HD3  | 1:662:A:LYS:HE3  | 12       | 0.28          |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 13       | 0.28          |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 20       | 0.28          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 14       | 0.28          |
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD13 | 1        | 0.28          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG21 | 16       | 0.27          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG22 | 16       | 0.27          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG23 | 16       | 0.27          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG21 | 16       | 0.27          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG22 | 16       | 0.27          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG23 | 16       | 0.27          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD11 | 10       | 0.27          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD12 | 10       | 0.27          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD13 | 10       | 0.27          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD11 | 10       | 0.27          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD12 | 10       | 0.27          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD13 | 10       | 0.27          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 6        | 0.27          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 6        | 0.27          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 6        | 0.27          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 6        | 0.27          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 6        | 0.27          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 6        | 0.27          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 6        | 0.27          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 6        | 0.27          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 6        | 0.27          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 2        | 0.27          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 6        | 0.27          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 7        | 0.27          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 8        | 0.27          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 12       | 0.27          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 16       | 0.27          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 17       | 0.27          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 13       | 0.27          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 16       | 0.27          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 1        | 0.27          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 1        | 0.27          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 1        | 0.27          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 4        | 0.27          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 4        | 0.27          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 4        | 0.27          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 18       | 0.27          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 18       | 0.27          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 18       | 0.27          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 11       | 0.27          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 11       | 0.27          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 11       | 0.27          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 19       | 0.27          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 19       | 0.27          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 19       | 0.27          |
| (2,127) | 2:542:B:PHE:HA   | 2:545:B:LEU:HB3  | 11       | 0.27          |
| (2,93)  | 2:534:B:PHE:HD1  | 2:534:B:PHE:HB3  | 16       | 0.27          |
| (2,93)  | 2:534:B:PHE:HD2  | 2:534:B:PHE:HB3  | 16       | 0.27          |
| (2,77)  | 2:547:B:SER:HB3  | 2:544:B:ALA:HA   | 3        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 4        | 0.27          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 4        | 0.27          |
| (2,72)   | 2:537:B:ILE:HB   | 2:534:B:PHE:HD1  | 7        | 0.27          |
| (2,72)   | 2:537:B:ILE:HB   | 2:534:B:PHE:HD2  | 7        | 0.27          |
| (1,1005) | 1:607:A:LEU:HD11 | 1:653:A:LEU:HD21 | 4        | 0.27          |
| (1,1005) | 1:607:A:LEU:HD11 | 1:653:A:LEU:HD22 | 4        | 0.27          |
| (1,1005) | 1:607:A:LEU:HD11 | 1:653:A:LEU:HD23 | 4        | 0.27          |
| (1,1005) | 1:607:A:LEU:HD12 | 1:653:A:LEU:HD21 | 4        | 0.27          |
| (1,1005) | 1:607:A:LEU:HD12 | 1:653:A:LEU:HD22 | 4        | 0.27          |
| (1,1005) | 1:607:A:LEU:HD12 | 1:653:A:LEU:HD23 | 4        | 0.27          |
| (1,1005) | 1:607:A:LEU:HD13 | 1:653:A:LEU:HD21 | 4        | 0.27          |
| (1,1005) | 1:607:A:LEU:HD13 | 1:653:A:LEU:HD22 | 4        | 0.27          |
| (1,1005) | 1:607:A:LEU:HD13 | 1:653:A:LEU:HD23 | 4        | 0.27          |
| (1,999)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 10       | 0.27          |
| (1,999)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 10       | 0.27          |
| (1,999)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 10       | 0.27          |
| (1,998)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 10       | 0.27          |
| (1,998)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 10       | 0.27          |
| (1,998)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 10       | 0.27          |
| (1,986)  | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 12       | 0.27          |
| (1,986)  | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 19       | 0.27          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 1        | 0.27          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 1        | 0.27          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 9        | 0.27          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 9        | 0.27          |
| (1,966)  | 1:661:A:GLN:H    | 1:660:A:ILE:HG22 | 10       | 0.27          |
| (1,951)  | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 19       | 0.27          |
| (1,937)  | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 11       | 0.27          |
| (1,936)  | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 2        | 0.27          |
| (1,936)  | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 6        | 0.27          |
| (1,936)  | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 9        | 0.27          |
| (1,931)  | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 3        | 0.27          |
| (1,903)  | 1:653:A:LEU:H    | 1:653:A:LEU:HD12 | 2        | 0.27          |
| (1,881)  | 1:648:A:GLU:H    | 1:643:A:ALA:HB1  | 4        | 0.27          |
| (1,881)  | 1:648:A:GLU:H    | 1:643:A:ALA:HB2  | 16       | 0.27          |
| (1,881)  | 1:648:A:GLU:H    | 1:643:A:ALA:HB1  | 18       | 0.27          |
| (1,881)  | 1:648:A:GLU:H    | 1:643:A:ALA:HB1  | 20       | 0.27          |
| (1,866)  | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 5        | 0.27          |
| (1,864)  | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 1        | 0.27          |
| (1,864)  | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 2        | 0.27          |
| (1,864)  | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 3        | 0.27          |
| (1,864)  | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 12       | 0.27          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,843) | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 12       | 0.27          |
| (1,805) | 1:621:A:LYS:H    | 1:621:A:LYS:HG3  | 11       | 0.27          |
| (1,805) | 1:621:A:LYS:H    | 1:621:A:LYS:HG3  | 14       | 0.27          |
| (1,723) | 1:609:A:GLN:H    | 1:608:A:VAL:HG13 | 10       | 0.27          |
| (1,711) | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 10       | 0.27          |
| (1,710) | 1:588:A:ARG:H    | 1:587:A:VAL:HG23 | 17       | 0.27          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD12 | 1        | 0.27          |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG21 | 8        | 0.27          |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD11 | 20       | 0.27          |
| (1,631) | 1:645:A:SER:HA   | 1:645:A:SER:HB2  | 6        | 0.27          |
| (1,631) | 1:645:A:SER:HA   | 1:645:A:SER:HB2  | 15       | 0.27          |
| (1,631) | 1:645:A:SER:HA   | 1:645:A:SER:HB2  | 20       | 0.27          |
| (1,598) | 1:595:A:VAL:HG21 | 1:592:A:HIS:HA   | 2        | 0.27          |
| (1,592) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HE2  | 1        | 0.27          |
| (1,582) | 1:599:A:LEU:HD23 | 1:599:A:LEU:HD12 | 16       | 0.27          |
| (1,580) | 1:599:A:LEU:HD12 | 1:599:A:LEU:HA   | 16       | 0.27          |
| (1,571) | 1:591:A:TRP:HD1  | 1:589:A:LYS:HA   | 3        | 0.27          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 12       | 0.27          |
| (1,475) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG11 | 7        | 0.27          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG21 | 19       | 0.27          |
| (1,402) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HA   | 7        | 0.27          |
| (1,349) | 1:610:A:ALA:HB1  | 1:657:A:ILE:HD12 | 4        | 0.27          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG13 | 16       | 0.27          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG11 | 20       | 0.27          |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 14       | 0.27          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 11       | 0.27          |
| (1,225) | 1:632:A:ALA:HB2  | 1:604:A:VAL:HG21 | 12       | 0.27          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 1        | 0.27          |
| (1,122) | 1:595:A:VAL:HG22 | 1:649:A:TYR:HE1  | 8        | 0.27          |
| (1,122) | 1:595:A:VAL:HG22 | 1:649:A:TYR:HE2  | 8        | 0.27          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD1  | 15       | 0.27          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD2  | 15       | 0.27          |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 3        | 0.27          |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 11       | 0.27          |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 14       | 0.27          |
| (1,23)  | 1:653:A:LEU:HB3  | 1:653:A:LEU:HD12 | 16       | 0.27          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG21 | 19       | 0.26          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG22 | 19       | 0.26          |
| (3,25)  | 1:631:A:TYR:HB2  | 2:537:B:ILE:HG23 | 19       | 0.26          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG21 | 19       | 0.26          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG22 | 19       | 0.26          |
| (3,25)  | 1:631:A:TYR:HB3  | 2:537:B:ILE:HG23 | 19       | 0.26          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE1  | 11       | 0.26          |
| (3,22)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HE2  | 11       | 0.26          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE1  | 11       | 0.26          |
| (3,22)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HE2  | 11       | 0.26          |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE1  | 11       | 0.26          |
| (3,22)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HE2  | 11       | 0.26          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 15       | 0.26          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 15       | 0.26          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 15       | 0.26          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 15       | 0.26          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 15       | 0.26          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 15       | 0.26          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 4        | 0.26          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 11       | 0.26          |
| (2,230) | 2:539:B:ASP:H    | 2:538:B:ALA:HA   | 13       | 0.26          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 4        | 0.26          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 5        | 0.26          |
| (2,219) | 2:533:B:ASP:H    | 2:533:B:ASP:HB3  | 1        | 0.26          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 3        | 0.26          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 17       | 0.26          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 5        | 0.26          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 8        | 0.26          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 11       | 0.26          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 14       | 0.26          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 19       | 0.26          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 9        | 0.26          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 17       | 0.26          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 5        | 0.26          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 5        | 0.26          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 5        | 0.26          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 10       | 0.26          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 10       | 0.26          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 10       | 0.26          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 15       | 0.26          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 15       | 0.26          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 15       | 0.26          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD21 | 4        | 0.26          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD22 | 4        | 0.26          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD23 | 4        | 0.26          |
| (2,143) | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 12       | 0.26          |
| (2,143) | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 12       | 0.26          |
| (2,143) | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 12       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,143)  | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 17       | 0.26          |
| (2,143)  | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 17       | 0.26          |
| (2,143)  | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 17       | 0.26          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 5        | 0.26          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 5        | 0.26          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 5        | 0.26          |
| (2,125)  | 2:545:B:LEU:HB2  | 2:542:B:PHE:HA   | 20       | 0.26          |
| (2,93)   | 2:534:B:PHE:HD1  | 2:534:B:PHE:HB3  | 5        | 0.26          |
| (2,93)   | 2:534:B:PHE:HD2  | 2:534:B:PHE:HB3  | 5        | 0.26          |
| (2,93)   | 2:534:B:PHE:HD1  | 2:534:B:PHE:HB3  | 13       | 0.26          |
| (2,93)   | 2:534:B:PHE:HD2  | 2:534:B:PHE:HB3  | 13       | 0.26          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 1        | 0.26          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 1        | 0.26          |
| (2,69)   | 2:534:B:PHE:HA   | 2:534:B:PHE:HD1  | 15       | 0.26          |
| (2,69)   | 2:534:B:PHE:HA   | 2:534:B:PHE:HD2  | 15       | 0.26          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 4        | 0.26          |
| (1,993)  | 1:619:A:ALA:HB1  | 1:612:A:PHE:HZ   | 14       | 0.26          |
| (1,993)  | 1:619:A:ALA:HB2  | 1:612:A:PHE:HZ   | 14       | 0.26          |
| (1,993)  | 1:619:A:ALA:HB3  | 1:612:A:PHE:HZ   | 14       | 0.26          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 4        | 0.26          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 4        | 0.26          |
| (1,942)  | 1:664:A:LEU:H    | 1:664:A:LEU:HD12 | 2        | 0.26          |
| (1,937)  | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 6        | 0.26          |
| (1,936)  | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 13       | 0.26          |
| (1,921)  | 1:659:A:LYS:H    | 1:659:A:LYS:HG3  | 7        | 0.26          |
| (1,915)  | 1:657:A:ILE:H    | 1:657:A:ILE:HD13 | 13       | 0.26          |
| (1,881)  | 1:648:A:GLU:H    | 1:643:A:ALA:HB3  | 10       | 0.26          |
| (1,866)  | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 16       | 0.26          |
| (1,864)  | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 6        | 0.26          |
| (1,864)  | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 15       | 0.26          |
| (1,843)  | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 11       | 0.26          |
| (1,783)  | 1:616:A:ASP:H    | 1:615:A:PRO:HD3  | 20       | 0.26          |
| (1,766)  | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 5        | 0.26          |
| (1,762)  | 1:605:A:HIS:H    | 1:604:A:VAL:HG21 | 10       | 0.26          |
| (1,717)  | 1:610:A:ALA:H    | 1:657:A:ILE:HD13 | 3        | 0.26          |
| (1,711)  | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 20       | 0.26          |
| (1,688)  | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 13       | 0.26          |
| (1,688)  | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 17       | 0.26          |
| (1,677)  | 1:643:A:ALA:H    | 1:642:A:SER:HB2  | 3        | 0.26          |
| (1,672)  | 1:593:A:GLU:H    | 1:593:A:GLU:HG2  | 17       | 0.26          |
| (1,665)  | 1:592:A:HIS:H    | 1:592:A:HIS:HB2  | 6        | 0.26          |
| (1,650)  | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 3        | 0.26          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,606) | 1:595:A:VAL:HA   | 1:599:A:LEU:HD23 | 10       | 0.26          |
| (1,592) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HE2  | 20       | 0.26          |
| (1,584) | 1:649:A:TYR:HE1  | 1:599:A:LEU:HD11 | 9        | 0.26          |
| (1,584) | 1:649:A:TYR:HE2  | 1:599:A:LEU:HD11 | 9        | 0.26          |
| (1,580) | 1:599:A:LEU:HD11 | 1:599:A:LEU:HA   | 14       | 0.26          |
| (1,572) | 1:654:A:ALA:HB3  | 1:657:A:ILE:HD11 | 7        | 0.26          |
| (1,572) | 1:654:A:ALA:HB3  | 1:657:A:ILE:HD11 | 18       | 0.26          |
| (1,524) | 1:595:A:VAL:HG21 | 1:646:A:ARG:HD3  | 13       | 0.26          |
| (1,475) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG13 | 20       | 0.26          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 13       | 0.26          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 2        | 0.26          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG21 | 16       | 0.26          |
| (1,412) | 1:630:A:ALA:HB3  | 1:627:A:ASN:HA   | 17       | 0.26          |
| (1,402) | 1:629:A:VAL:HG11 | 1:630:A:ALA:HA   | 12       | 0.26          |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG13 | 18       | 0.26          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG12 | 14       | 0.26          |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD23 | 4        | 0.26          |
| (1,349) | 1:610:A:ALA:HB1  | 1:657:A:ILE:HD13 | 18       | 0.26          |
| (1,337) | 1:611:A:ILE:HD11 | 1:611:A:ILE:HB   | 10       | 0.26          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG11 | 6        | 0.26          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 3        | 0.26          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 5        | 0.26          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 7        | 0.26          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 15       | 0.26          |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG23 | 8        | 0.26          |
| (1,224) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HG21 | 2        | 0.26          |
| (1,209) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD22 | 14       | 0.26          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 5        | 0.26          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 4        | 0.26          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 8        | 0.26          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 9        | 0.26          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 16       | 0.26          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 18       | 0.26          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 20       | 0.26          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB2  | 18       | 0.26          |
| (1,122) | 1:595:A:VAL:HG23 | 1:649:A:TYR:HE1  | 4        | 0.26          |
| (1,122) | 1:595:A:VAL:HG23 | 1:649:A:TYR:HE2  | 4        | 0.26          |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 4        | 0.26          |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 6        | 0.26          |
| (1,65)  | 1:617:A:PRO:HG2  | 1:616:A:ASP:HA   | 7        | 0.26          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 11       | 0.26          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 12       | 0.26          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD11 | 5        | 0.26          |
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD11 | 6        | 0.26          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD21 | 5        | 0.25          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD22 | 5        | 0.25          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD23 | 5        | 0.25          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD21 | 5        | 0.25          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD22 | 5        | 0.25          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD23 | 5        | 0.25          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 14       | 0.25          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 14       | 0.25          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 14       | 0.25          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 14       | 0.25          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 14       | 0.25          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 14       | 0.25          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 1        | 0.25          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 2        | 0.25          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 6        | 0.25          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 8        | 0.25          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 9        | 0.25          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 10       | 0.25          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 12       | 0.25          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 14       | 0.25          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 15       | 0.25          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 16       | 0.25          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 17       | 0.25          |
| (2,225) | 2:542:B:PHE:H    | 2:541:B:ASP:HA   | 18       | 0.25          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 1        | 0.25          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 14       | 0.25          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 18       | 0.25          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 6        | 0.25          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 10       | 0.25          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 12       | 0.25          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD11 | 3        | 0.25          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD12 | 3        | 0.25          |
| (2,146) | 2:545:B:LEU:HA   | 2:545:B:LEU:HD13 | 3        | 0.25          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD21 | 10       | 0.25          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD22 | 10       | 0.25          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD23 | 10       | 0.25          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 13       | 0.25          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 13       | 0.25          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 13       | 0.25          |
| (2,141) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 18       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 18       | 0.25          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 18       | 0.25          |
| (2,137)  | 2:543:B:SER:HA   | 2:546:B:LEU:HB2  | 10       | 0.25          |
| (2,137)  | 2:543:B:SER:HA   | 2:546:B:LEU:HB2  | 16       | 0.25          |
| (2,93)   | 2:534:B:PHE:HD1  | 2:534:B:PHE:HB3  | 12       | 0.25          |
| (2,93)   | 2:534:B:PHE:HD2  | 2:534:B:PHE:HB3  | 12       | 0.25          |
| (2,77)   | 2:547:B:SER:HB3  | 2:544:B:ALA:HA   | 15       | 0.25          |
| (2,72)   | 2:537:B:ILE:HB   | 2:534:B:PHE:HD1  | 19       | 0.25          |
| (2,72)   | 2:537:B:ILE:HB   | 2:534:B:PHE:HD2  | 19       | 0.25          |
| (2,49)   | 2:537:B:ILE:HD11 | 2:537:B:ILE:HA   | 20       | 0.25          |
| (2,49)   | 2:537:B:ILE:HD12 | 2:537:B:ILE:HA   | 20       | 0.25          |
| (2,49)   | 2:537:B:ILE:HD13 | 2:537:B:ILE:HA   | 20       | 0.25          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 15       | 0.25          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 15       | 0.25          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 15       | 0.25          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB1  | 1        | 0.25          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB2  | 1        | 0.25          |
| (1,1016) | 1:591:A:TRP:HH2  | 1:643:A:ALA:HB3  | 1        | 0.25          |
| (1,986)  | 1:660:A:ILE:H    | 1:659:A:LYS:HG3  | 18       | 0.25          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 14       | 0.25          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 14       | 0.25          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 15       | 0.25          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 15       | 0.25          |
| (1,971)  | 1:627:A:ASN:H    | 1:626:A:GLU:HB2  | 19       | 0.25          |
| (1,966)  | 1:661:A:GLN:H    | 1:660:A:ILE:HG23 | 14       | 0.25          |
| (1,952)  | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 5        | 0.25          |
| (1,937)  | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 12       | 0.25          |
| (1,936)  | 1:663:A:GLU:H    | 1:663:A:GLU:HB3  | 16       | 0.25          |
| (1,925)  | 1:660:A:ILE:H    | 1:660:A:ILE:HD12 | 6        | 0.25          |
| (1,921)  | 1:659:A:LYS:H    | 1:659:A:LYS:HG3  | 11       | 0.25          |
| (1,915)  | 1:657:A:ILE:H    | 1:657:A:ILE:HD13 | 5        | 0.25          |
| (1,881)  | 1:648:A:GLU:H    | 1:643:A:ALA:HB2  | 1        | 0.25          |
| (1,881)  | 1:648:A:GLU:H    | 1:643:A:ALA:HB3  | 5        | 0.25          |
| (1,881)  | 1:648:A:GLU:H    | 1:643:A:ALA:HB3  | 6        | 0.25          |
| (1,881)  | 1:648:A:GLU:H    | 1:643:A:ALA:HB3  | 11       | 0.25          |
| (1,881)  | 1:648:A:GLU:H    | 1:643:A:ALA:HB3  | 12       | 0.25          |
| (1,881)  | 1:648:A:GLU:H    | 1:643:A:ALA:HB2  | 14       | 0.25          |
| (1,864)  | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 7        | 0.25          |
| (1,864)  | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 8        | 0.25          |
| (1,864)  | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 10       | 0.25          |
| (1,850)  | 1:634:A:LYS:H    | 1:634:A:LYS:HB3  | 8        | 0.25          |
| (1,762)  | 1:605:A:HIS:H    | 1:604:A:VAL:HG23 | 1        | 0.25          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,723) | 1:609:A:GLN:H    | 1:608:A:VAL:HG11 | 3        | 0.25          |
| (1,723) | 1:609:A:GLN:H    | 1:608:A:VAL:HG12 | 6        | 0.25          |
| (1,711) | 1:589:A:LYS:H    | 1:589:A:LYS:HD2  | 14       | 0.25          |
| (1,695) | 1:641:A:GLU:H    | 1:641:A:GLU:HG2  | 17       | 0.25          |
| (1,688) | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 1        | 0.25          |
| (1,688) | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 6        | 0.25          |
| (1,688) | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 7        | 0.25          |
| (1,688) | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 8        | 0.25          |
| (1,688) | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 9        | 0.25          |
| (1,688) | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 10       | 0.25          |
| (1,688) | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 19       | 0.25          |
| (1,677) | 1:643:A:ALA:H    | 1:642:A:SER:HB2  | 2        | 0.25          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD13 | 13       | 0.25          |
| (1,665) | 1:592:A:HIS:H    | 1:592:A:HIS:HB2  | 16       | 0.25          |
| (1,657) | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE1  | 2        | 0.25          |
| (1,657) | 1:595:A:VAL:HG13 | 1:649:A:TYR:HE2  | 2        | 0.25          |
| (1,624) | 1:631:A:TYR:HD1  | 1:628:A:LEU:HD11 | 11       | 0.25          |
| (1,624) | 1:631:A:TYR:HD2  | 1:628:A:LEU:HD11 | 11       | 0.25          |
| (1,582) | 1:599:A:LEU:HD21 | 1:599:A:LEU:HD13 | 1        | 0.25          |
| (1,580) | 1:599:A:LEU:HD11 | 1:599:A:LEU:HA   | 10       | 0.25          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 2        | 0.25          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 9        | 0.25          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 10       | 0.25          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 20       | 0.25          |
| (1,456) | 1:608:A:VAL:HB   | 1:605:A:HIS:HA   | 1        | 0.25          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 5        | 0.25          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG21 | 7        | 0.25          |
| (1,412) | 1:630:A:ALA:HB1  | 1:627:A:ASN:HA   | 1        | 0.25          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 8        | 0.25          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 10       | 0.25          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 13       | 0.25          |
| (1,402) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HA   | 6        | 0.25          |
| (1,376) | 1:633:A:LYS:HD3  | 1:604:A:VAL:HG12 | 19       | 0.25          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG21 | 8        | 0.25          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 12       | 0.25          |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 6        | 0.25          |
| (1,224) | 1:604:A:VAL:HG11 | 1:604:A:VAL:HG22 | 6        | 0.25          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 20       | 0.25          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE1  | 10       | 0.25          |
| (1,121) | 1:653:A:LEU:HD11 | 1:649:A:TYR:HE2  | 10       | 0.25          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD1  | 2        | 0.25          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD2  | 2        | 0.25          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,93)  | 1:662:A:LYS:HG3 | 1:662:A:LYS:HE2  | 7        | 0.25          |
| (1,91)  | 1:662:A:LYS:HG2 | 1:662:A:LYS:HE2  | 17       | 0.25          |
| (1,91)  | 1:662:A:LYS:HG2 | 1:662:A:LYS:HE2  | 18       | 0.25          |
| (1,91)  | 1:662:A:LYS:HG2 | 1:662:A:LYS:HE2  | 19       | 0.25          |
| (1,2)   | 1:639:A:MET:HG2 | 1:639:A:MET:HE3  | 20       | 0.25          |
| (3,10)  | 1:624:A:ARG:HB2 | 2:545:B:LEU:HD11 | 6        | 0.24          |
| (3,10)  | 1:624:A:ARG:HB2 | 2:545:B:LEU:HD12 | 6        | 0.24          |
| (3,10)  | 1:624:A:ARG:HB2 | 2:545:B:LEU:HD13 | 6        | 0.24          |
| (3,10)  | 1:624:A:ARG:HB3 | 2:545:B:LEU:HD11 | 6        | 0.24          |
| (3,10)  | 1:624:A:ARG:HB3 | 2:545:B:LEU:HD12 | 6        | 0.24          |
| (3,10)  | 1:624:A:ARG:HB3 | 2:545:B:LEU:HD13 | 6        | 0.24          |
| (3,9)   | 1:619:A:ALA:HB1 | 2:545:B:LEU:HD21 | 9        | 0.24          |
| (3,9)   | 1:619:A:ALA:HB1 | 2:545:B:LEU:HD22 | 9        | 0.24          |
| (3,9)   | 1:619:A:ALA:HB1 | 2:545:B:LEU:HD23 | 9        | 0.24          |
| (3,9)   | 1:619:A:ALA:HB2 | 2:545:B:LEU:HD21 | 9        | 0.24          |
| (3,9)   | 1:619:A:ALA:HB2 | 2:545:B:LEU:HD22 | 9        | 0.24          |
| (3,9)   | 1:619:A:ALA:HB2 | 2:545:B:LEU:HD23 | 9        | 0.24          |
| (3,9)   | 1:619:A:ALA:HB3 | 2:545:B:LEU:HD21 | 9        | 0.24          |
| (3,9)   | 1:619:A:ALA:HB3 | 2:545:B:LEU:HD22 | 9        | 0.24          |
| (3,9)   | 1:619:A:ALA:HB3 | 2:545:B:LEU:HD23 | 9        | 0.24          |
| (3,5)   | 1:612:A:PHE:HB2 | 2:545:B:LEU:HD21 | 1        | 0.24          |
| (3,5)   | 1:612:A:PHE:HB2 | 2:545:B:LEU:HD22 | 1        | 0.24          |
| (3,5)   | 1:612:A:PHE:HB2 | 2:545:B:LEU:HD23 | 1        | 0.24          |
| (3,5)   | 1:612:A:PHE:HB3 | 2:545:B:LEU:HD21 | 1        | 0.24          |
| (3,5)   | 1:612:A:PHE:HB3 | 2:545:B:LEU:HD22 | 1        | 0.24          |
| (3,5)   | 1:612:A:PHE:HB3 | 2:545:B:LEU:HD23 | 1        | 0.24          |
| (2,225) | 2:542:B:PHE:H   | 2:541:B:ASP:HA   | 11       | 0.24          |
| (2,225) | 2:542:B:PHE:H   | 2:541:B:ASP:HA   | 13       | 0.24          |
| (2,225) | 2:542:B:PHE:H   | 2:541:B:ASP:HA   | 20       | 0.24          |
| (2,196) | 2:541:B:ASP:H   | 2:541:B:ASP:HB3  | 4        | 0.24          |
| (2,196) | 2:541:B:ASP:H   | 2:541:B:ASP:HB3  | 6        | 0.24          |
| (2,196) | 2:541:B:ASP:H   | 2:541:B:ASP:HB3  | 7        | 0.24          |
| (2,151) | 2:546:B:LEU:HB2 | 2:547:B:SER:HA   | 7        | 0.24          |
| (2,93)  | 2:534:B:PHE:HD1 | 2:534:B:PHE:HB3  | 7        | 0.24          |
| (2,93)  | 2:534:B:PHE:HD2 | 2:534:B:PHE:HB3  | 7        | 0.24          |
| (2,93)  | 2:534:B:PHE:HD1 | 2:534:B:PHE:HB3  | 11       | 0.24          |
| (2,93)  | 2:534:B:PHE:HD2 | 2:534:B:PHE:HB3  | 11       | 0.24          |
| (1,993) | 1:619:A:ALA:HB1 | 1:612:A:PHE:HZ   | 1        | 0.24          |
| (1,993) | 1:619:A:ALA:HB2 | 1:612:A:PHE:HZ   | 1        | 0.24          |
| (1,993) | 1:619:A:ALA:HB3 | 1:612:A:PHE:HZ   | 1        | 0.24          |
| (1,979) | 1:612:A:PHE:H   | 1:612:A:PHE:HD1  | 6        | 0.24          |
| (1,979) | 1:612:A:PHE:H   | 1:612:A:PHE:HD2  | 6        | 0.24          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 11       | 0.24          |
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 11       | 0.24          |
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 13       | 0.24          |
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 13       | 0.24          |
| (1,966) | 1:661:A:GLN:H    | 1:660:A:ILE:HG22 | 1        | 0.24          |
| (1,966) | 1:661:A:GLN:H    | 1:660:A:ILE:HG22 | 9        | 0.24          |
| (1,903) | 1:653:A:LEU:H    | 1:653:A:LEU:HD11 | 15       | 0.24          |
| (1,881) | 1:648:A:GLU:H    | 1:643:A:ALA:HB2  | 2        | 0.24          |
| (1,881) | 1:648:A:GLU:H    | 1:643:A:ALA:HB1  | 3        | 0.24          |
| (1,881) | 1:648:A:GLU:H    | 1:643:A:ALA:HB1  | 7        | 0.24          |
| (1,881) | 1:648:A:GLU:H    | 1:643:A:ALA:HB1  | 8        | 0.24          |
| (1,881) | 1:648:A:GLU:H    | 1:643:A:ALA:HB2  | 19       | 0.24          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD1  | 2        | 0.24          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD2  | 2        | 0.24          |
| (1,732) | 1:594:A:HIS:H    | 1:593:A:GLU:HB3  | 7        | 0.24          |
| (1,723) | 1:609:A:GLN:H    | 1:608:A:VAL:HG12 | 8        | 0.24          |
| (1,688) | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 2        | 0.24          |
| (1,688) | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 5        | 0.24          |
| (1,650) | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 5        | 0.24          |
| (1,582) | 1:599:A:LEU:HD22 | 1:599:A:LEU:HD11 | 12       | 0.24          |
| (1,582) | 1:599:A:LEU:HD23 | 1:599:A:LEU:HD12 | 20       | 0.24          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 3        | 0.24          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 5        | 0.24          |
| (1,503) | 1:625:A:MET:HG2  | 1:629:A:VAL:HG21 | 14       | 0.24          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD23 | 3        | 0.24          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD21 | 7        | 0.24          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD21 | 12       | 0.24          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 18       | 0.24          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG22 | 1        | 0.24          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG23 | 5        | 0.24          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG22 | 17       | 0.24          |
| (1,402) | 1:629:A:VAL:HG12 | 1:630:A:ALA:HA   | 9        | 0.24          |
| (1,394) | 1:635:A:VAL:HG12 | 1:632:A:ALA:HA   | 18       | 0.24          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 13       | 0.24          |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 4        | 0.24          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 5        | 0.24          |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG23 | 20       | 0.24          |
| (1,225) | 1:632:A:ALA:HB2  | 1:604:A:VAL:HG22 | 9        | 0.24          |
| (1,225) | 1:632:A:ALA:HB3  | 1:604:A:VAL:HG23 | 18       | 0.24          |
| (1,224) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HG21 | 12       | 0.24          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 6        | 0.24          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 10       | 0.24          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 11       | 0.24          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 13       | 0.24          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 12       | 0.24          |
| (1,118) | 1:653:A:LEU:HB3  | 1:650:A:TYR:HA   | 12       | 0.24          |
| (1,93)  | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE2  | 11       | 0.24          |
| (1,21)  | 1:664:A:LEU:HD22 | 1:664:A:LEU:HD11 | 8        | 0.24          |
| (3,32)  | 1:664:A:LEU:HD11 | 2:542:B:PHE:HE1  | 13       | 0.23          |
| (3,32)  | 1:664:A:LEU:HD11 | 2:542:B:PHE:HE2  | 13       | 0.23          |
| (3,32)  | 1:664:A:LEU:HD12 | 2:542:B:PHE:HE1  | 13       | 0.23          |
| (3,32)  | 1:664:A:LEU:HD12 | 2:542:B:PHE:HE2  | 13       | 0.23          |
| (3,32)  | 1:664:A:LEU:HD13 | 2:542:B:PHE:HE1  | 13       | 0.23          |
| (3,32)  | 1:664:A:LEU:HD13 | 2:542:B:PHE:HE2  | 13       | 0.23          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD1  | 2        | 0.23          |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD2  | 2        | 0.23          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD1  | 2        | 0.23          |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD2  | 2        | 0.23          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD1  | 2        | 0.23          |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD2  | 2        | 0.23          |
| (3,18)  | 1:627:A:ASN:HB2  | 2:537:B:ILE:HG21 | 12       | 0.23          |
| (3,18)  | 1:627:A:ASN:HB2  | 2:537:B:ILE:HG22 | 12       | 0.23          |
| (3,18)  | 1:627:A:ASN:HB2  | 2:537:B:ILE:HG23 | 12       | 0.23          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD21 | 4        | 0.23          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD22 | 4        | 0.23          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD23 | 4        | 0.23          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD21 | 4        | 0.23          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD22 | 4        | 0.23          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD23 | 4        | 0.23          |
| (2,250) | 2:534:B:PHE:H    | 2:534:B:PHE:HD1  | 20       | 0.23          |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 7        | 0.23          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 10       | 0.23          |
| (2,185) | 2:540:B:MET:HG3  | 2:540:B:MET:HB3  | 17       | 0.23          |
| (2,185) | 2:540:B:MET:HG3  | 2:540:B:MET:HB3  | 18       | 0.23          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 1        | 0.23          |
| (2,169) | 2:544:B:ALA:HA   | 2:547:B:SER:HB3  | 6        | 0.23          |
| (2,169) | 2:544:B:ALA:HA   | 2:547:B:SER:HB3  | 11       | 0.23          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 8        | 0.23          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 13       | 0.23          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD21 | 16       | 0.23          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD22 | 16       | 0.23          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD23 | 16       | 0.23          |
| (2,143) | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 2        | 0.23          |
| (2,143) | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 2        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,143)  | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 2        | 0.23          |
| (2,143)  | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 14       | 0.23          |
| (2,143)  | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 14       | 0.23          |
| (2,143)  | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 14       | 0.23          |
| (2,137)  | 2:543:B:SER:HA   | 2:546:B:LEU:HB2  | 4        | 0.23          |
| (2,127)  | 2:542:B:PHE:HA   | 2:545:B:LEU:HB3  | 18       | 0.23          |
| (2,121)  | 2:540:B:MET:HA   | 2:540:B:MET:HG2  | 20       | 0.23          |
| (2,76)   | 2:542:B:PHE:HA   | 2:542:B:PHE:HD1  | 18       | 0.23          |
| (2,76)   | 2:542:B:PHE:HA   | 2:542:B:PHE:HD2  | 18       | 0.23          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 10       | 0.23          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 10       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD1  | 10       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD2  | 10       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD1  | 10       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD2  | 10       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD1  | 10       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD2  | 10       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD1  | 16       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD2  | 16       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD1  | 16       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD2  | 16       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD1  | 16       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD2  | 16       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD1  | 18       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD11 | 1:650:A:TYR:HD2  | 18       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD1  | 18       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD12 | 1:650:A:TYR:HD2  | 18       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD1  | 18       | 0.23          |
| (1,1013) | 1:599:A:LEU:HD13 | 1:650:A:TYR:HD2  | 18       | 0.23          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 18       | 0.23          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 18       | 0.23          |
| (1,966)  | 1:661:A:GLN:H    | 1:660:A:ILE:HG23 | 2        | 0.23          |
| (1,966)  | 1:661:A:GLN:H    | 1:660:A:ILE:HG22 | 4        | 0.23          |
| (1,966)  | 1:661:A:GLN:H    | 1:660:A:ILE:HG22 | 15       | 0.23          |
| (1,951)  | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 3        | 0.23          |
| (1,944)  | 1:666:A:GLU:H    | 1:666:A:GLU:HG2  | 12       | 0.23          |
| (1,915)  | 1:657:A:ILE:H    | 1:657:A:ILE:HD13 | 10       | 0.23          |
| (1,866)  | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 19       | 0.23          |
| (1,785)  | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 18       | 0.23          |
| (1,732)  | 1:594:A:HIS:H    | 1:593:A:GLU:HB3  | 4        | 0.23          |
| (1,732)  | 1:594:A:HIS:H    | 1:593:A:GLU:HB3  | 18       | 0.23          |
| (1,723)  | 1:609:A:GLN:H    | 1:608:A:VAL:HG12 | 18       | 0.23          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,688) | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 20       | 0.23          |
| (1,657) | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE1  | 16       | 0.23          |
| (1,657) | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE2  | 16       | 0.23          |
| (1,650) | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 13       | 0.23          |
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD11 | 14       | 0.23          |
| (1,630) | 1:628:A:LEU:HB3  | 1:628:A:LEU:HD11 | 3        | 0.23          |
| (1,606) | 1:595:A:VAL:HA   | 1:599:A:LEU:HD22 | 14       | 0.23          |
| (1,582) | 1:599:A:LEU:HD21 | 1:599:A:LEU:HD12 | 3        | 0.23          |
| (1,582) | 1:599:A:LEU:HD23 | 1:599:A:LEU:HD13 | 10       | 0.23          |
| (1,572) | 1:654:A:ALA:HB1  | 1:657:A:ILE:HD11 | 16       | 0.23          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 16       | 0.23          |
| (1,503) | 1:625:A:MET:HG2  | 1:629:A:VAL:HG22 | 11       | 0.23          |
| (1,475) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG11 | 2        | 0.23          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD22 | 6        | 0.23          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 20       | 0.23          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 16       | 0.23          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG21 | 13       | 0.23          |
| (1,412) | 1:630:A:ALA:HB1  | 1:627:A:ASN:HA   | 5        | 0.23          |
| (1,412) | 1:630:A:ALA:HB2  | 1:627:A:ASN:HA   | 18       | 0.23          |
| (1,412) | 1:630:A:ALA:HB3  | 1:627:A:ASN:HA   | 19       | 0.23          |
| (1,402) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HA   | 11       | 0.23          |
| (1,402) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HA   | 16       | 0.23          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG23 | 15       | 0.23          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 12       | 0.23          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG11 | 4        | 0.23          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG12 | 13       | 0.23          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG13 | 17       | 0.23          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 6        | 0.23          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 10       | 0.23          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 11       | 0.23          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 13       | 0.23          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 15       | 0.23          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 17       | 0.23          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 18       | 0.23          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 19       | 0.23          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 16       | 0.23          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 15       | 0.23          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 20       | 0.23          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 3        | 0.23          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 13       | 0.23          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 16       | 0.23          |
| (1,224) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HG21 | 11       | 0.23          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 1        | 0.23          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 2        | 0.23          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 3        | 0.23          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 4        | 0.23          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 15       | 0.23          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 17       | 0.23          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 18       | 0.23          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 20       | 0.23          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 2        | 0.23          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 1        | 0.23          |
| (1,156) | 1:602:A:HIS:HA   | 1:605:A:HIS:HB3  | 2        | 0.23          |
| (1,122) | 1:595:A:VAL:HG21 | 1:649:A:TYR:HE1  | 7        | 0.23          |
| (1,122) | 1:595:A:VAL:HG21 | 1:649:A:TYR:HE2  | 7        | 0.23          |
| (1,91)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HE2  | 2        | 0.23          |
| (1,91)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HE2  | 10       | 0.23          |
| (1,71)  | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 4        | 0.23          |
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD13 | 2        | 0.23          |
| (1,21)  | 1:664:A:LEU:HD23 | 1:664:A:LEU:HD13 | 7        | 0.23          |
| (3,18)  | 1:627:A:ASN:HB2  | 2:537:B:ILE:HG21 | 6        | 0.22          |
| (3,18)  | 1:627:A:ASN:HB2  | 2:537:B:ILE:HG22 | 6        | 0.22          |
| (3,18)  | 1:627:A:ASN:HB2  | 2:537:B:ILE:HG23 | 6        | 0.22          |
| (2,256) | 2:538:B:ALA:H    | 2:537:B:ILE:HG22 | 11       | 0.22          |
| (2,240) | 2:542:B:PHE:H    | 2:542:B:PHE:HB2  | 3        | 0.22          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 5        | 0.22          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 19       | 0.22          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 20       | 0.22          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 5        | 0.22          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD21 | 20       | 0.22          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD22 | 20       | 0.22          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD23 | 20       | 0.22          |
| (2,143) | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 8        | 0.22          |
| (2,143) | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 8        | 0.22          |
| (2,143) | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 8        | 0.22          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 20       | 0.22          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 7        | 0.22          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 7        | 0.22          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 20       | 0.22          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 3        | 0.22          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 3        | 0.22          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 3        | 0.22          |
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 5        | 0.22          |
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 5        | 0.22          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 17       | 0.22          |
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 17       | 0.22          |
| (1,931) | 1:662:A:LYS:H    | 1:661:A:GLN:HB3  | 19       | 0.22          |
| (1,915) | 1:657:A:ILE:H    | 1:657:A:ILE:HD12 | 20       | 0.22          |
| (1,912) | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 2        | 0.22          |
| (1,866) | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 4        | 0.22          |
| (1,843) | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 4        | 0.22          |
| (1,843) | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 13       | 0.22          |
| (1,778) | 1:611:A:ILE:H    | 1:611:A:ILE:HG12 | 6        | 0.22          |
| (1,778) | 1:611:A:ILE:H    | 1:611:A:ILE:HG12 | 11       | 0.22          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 1        | 0.22          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 10       | 0.22          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 18       | 0.22          |
| (1,766) | 1:606:A:LYS:H    | 1:607:A:LEU:HB2  | 19       | 0.22          |
| (1,732) | 1:594:A:HIS:H    | 1:593:A:GLU:HB3  | 14       | 0.22          |
| (1,723) | 1:609:A:GLN:H    | 1:608:A:VAL:HG12 | 4        | 0.22          |
| (1,592) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HE2  | 5        | 0.22          |
| (1,580) | 1:599:A:LEU:HD13 | 1:599:A:LEU:HA   | 13       | 0.22          |
| (1,572) | 1:654:A:ALA:HB3  | 1:657:A:ILE:HD13 | 13       | 0.22          |
| (1,504) | 1:629:A:VAL:HG12 | 1:629:A:VAL:HG23 | 3        | 0.22          |
| (1,504) | 1:629:A:VAL:HG12 | 1:629:A:VAL:HG23 | 12       | 0.22          |
| (1,504) | 1:629:A:VAL:HG13 | 1:629:A:VAL:HG22 | 20       | 0.22          |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD22 | 18       | 0.22          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD22 | 1        | 0.22          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD22 | 5        | 0.22          |
| (1,464) | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 15       | 0.22          |
| (1,461) | 1:656:A:LYS:HD3  | 1:656:A:LYS:HA   | 10       | 0.22          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 19       | 0.22          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 7        | 0.22          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG23 | 3        | 0.22          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG23 | 10       | 0.22          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG21 | 20       | 0.22          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 4        | 0.22          |
| (1,402) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HA   | 4        | 0.22          |
| (1,402) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HA   | 10       | 0.22          |
| (1,402) | 1:629:A:VAL:HG12 | 1:630:A:ALA:HA   | 20       | 0.22          |
| (1,392) | 1:635:A:VAL:HG22 | 1:632:A:ALA:HA   | 14       | 0.22          |
| (1,392) | 1:635:A:VAL:HG23 | 1:632:A:ALA:HA   | 15       | 0.22          |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG12 | 15       | 0.22          |
| (1,367) | 1:653:A:LEU:HB2  | 1:653:A:LEU:HD22 | 7        | 0.22          |
| (1,364) | 1:648:A:GLU:HA   | 1:651:A:HIS:HB2  | 10       | 0.22          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 4        | 0.22          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 7        | 0.22          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 8        | 0.22          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 13       | 0.22          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 15       | 0.22          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 16       | 0.22          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 2        | 0.22          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 20       | 0.22          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 9        | 0.22          |
| (1,268) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HB3  | 12       | 0.22          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 19       | 0.22          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 8        | 0.22          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 10       | 0.22          |
| (1,225) | 1:632:A:ALA:HB2  | 1:604:A:VAL:HG21 | 11       | 0.22          |
| (1,224) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HG22 | 9        | 0.22          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 7        | 0.22          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 8        | 0.22          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 9        | 0.22          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 12       | 0.22          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 14       | 0.22          |
| (1,196) | 1:622:A:ASP:HB3  | 1:622:A:ASP:HA   | 16       | 0.22          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 8        | 0.22          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 10       | 0.22          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 13       | 0.22          |
| (1,97)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HD3  | 16       | 0.22          |
| (1,93)  | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE2  | 1        | 0.22          |
| (1,71)  | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 9        | 0.22          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 16       | 0.22          |
| (1,63)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HB2  | 20       | 0.22          |
| (1,42)  | 1:597:A:GLN:HG2  | 1:597:A:GLN:HA   | 15       | 0.22          |
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD11 | 9        | 0.22          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD11 | 20       | 0.21          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD12 | 20       | 0.21          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD13 | 20       | 0.21          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD11 | 20       | 0.21          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD12 | 20       | 0.21          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD13 | 20       | 0.21          |
| (2,252) | 2:535:B:SER:H    | 2:534:B:PHE:HD1  | 5        | 0.21          |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 4        | 0.21          |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 13       | 0.21          |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 4        | 0.21          |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 12       | 0.21          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 18       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,144)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD21 | 3        | 0.21          |
| (2,144)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD22 | 3        | 0.21          |
| (2,144)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD23 | 3        | 0.21          |
| (2,143)  | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 11       | 0.21          |
| (2,143)  | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 11       | 0.21          |
| (2,143)  | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 11       | 0.21          |
| (2,143)  | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 15       | 0.21          |
| (2,143)  | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 15       | 0.21          |
| (2,143)  | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 15       | 0.21          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 4        | 0.21          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 4        | 0.21          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 4        | 0.21          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 10       | 0.21          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 10       | 0.21          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 10       | 0.21          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD11 | 16       | 0.21          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD12 | 16       | 0.21          |
| (2,141)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD13 | 16       | 0.21          |
| (2,127)  | 2:542:B:PHE:HA   | 2:545:B:LEU:HB3  | 14       | 0.21          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 2        | 0.21          |
| (2,74)   | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 2        | 0.21          |
| (1,1010) | 1:641:A:GLU:HA   | 1:591:A:TRP:HZ2  | 8        | 0.21          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG11 | 16       | 0.21          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG12 | 16       | 0.21          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG13 | 16       | 0.21          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG11 | 16       | 0.21          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG12 | 16       | 0.21          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG13 | 16       | 0.21          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG11 | 16       | 0.21          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG12 | 16       | 0.21          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG13 | 16       | 0.21          |
| (1,937)  | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 4        | 0.21          |
| (1,915)  | 1:657:A:ILE:H    | 1:657:A:ILE:HD11 | 7        | 0.21          |
| (1,866)  | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 3        | 0.21          |
| (1,866)  | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 11       | 0.21          |
| (1,864)  | 1:638:A:ASP:H    | 1:638:A:ASP:HB3  | 17       | 0.21          |
| (1,785)  | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 19       | 0.21          |
| (1,785)  | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 20       | 0.21          |
| (1,732)  | 1:594:A:HIS:H    | 1:593:A:GLU:HB3  | 5        | 0.21          |
| (1,723)  | 1:609:A:GLN:H    | 1:608:A:VAL:HG13 | 14       | 0.21          |
| (1,688)  | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 3        | 0.21          |
| (1,688)  | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 11       | 0.21          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG23 | 10       | 0.21          |
| (1,605) | 1:602:A:HIS:HD2  | 1:599:A:LEU:HD23 | 1        | 0.21          |
| (1,583) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD12 | 8        | 0.21          |
| (1,582) | 1:599:A:LEU:HD23 | 1:599:A:LEU:HD13 | 6        | 0.21          |
| (1,582) | 1:599:A:LEU:HD22 | 1:599:A:LEU:HD11 | 19       | 0.21          |
| (1,572) | 1:654:A:ALA:HB2  | 1:657:A:ILE:HD12 | 20       | 0.21          |
| (1,548) | 1:603:A:LEU:HA   | 1:606:A:LYS:HD2  | 18       | 0.21          |
| (1,523) | 1:595:A:VAL:HG22 | 1:646:A:ARG:HD2  | 13       | 0.21          |
| (1,504) | 1:629:A:VAL:HG11 | 1:629:A:VAL:HG23 | 4        | 0.21          |
| (1,504) | 1:629:A:VAL:HG11 | 1:629:A:VAL:HG21 | 11       | 0.21          |
| (1,504) | 1:629:A:VAL:HG12 | 1:629:A:VAL:HG23 | 14       | 0.21          |
| (1,475) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG12 | 19       | 0.21          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD23 | 4        | 0.21          |
| (1,457) | 1:608:A:VAL:HG23 | 1:605:A:HIS:HA   | 12       | 0.21          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG21 | 4        | 0.21          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG21 | 9        | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 1        | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 2        | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 4        | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 5        | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 7        | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 8        | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 9        | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 10       | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 11       | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 12       | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 13       | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 14       | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 16       | 0.21          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 17       | 0.21          |
| (1,366) | 1:639:A:MET:HE2  | 1:653:A:LEU:HD21 | 16       | 0.21          |
| (1,364) | 1:648:A:GLU:HA   | 1:651:A:HIS:HB2  | 1        | 0.21          |
| (1,364) | 1:648:A:GLU:HA   | 1:651:A:HIS:HB2  | 14       | 0.21          |
| (1,349) | 1:610:A:ALA:HB2  | 1:657:A:ILE:HD12 | 13       | 0.21          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 5        | 0.21          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 19       | 0.21          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 7        | 0.21          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 1        | 0.21          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 10       | 0.21          |
| (1,281) | 1:668:A:ARG:HB3  | 1:668:A:ARG:HD2  | 11       | 0.21          |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 9        | 0.21          |
| (1,268) | 1:667:A:LYS:HD2  | 1:667:A:LYS:HB3  | 7        | 0.21          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,258) | 1:656:A:LYS:HA   | 1:659:A:LYS:HB3  | 13       | 0.21          |
| (1,256) | 1:659:A:LYS:HB2  | 1:659:A:LYS:HG2  | 4        | 0.21          |
| (1,118) | 1:653:A:LEU:HB3  | 1:650:A:TYR:HA   | 19       | 0.21          |
| (1,101) | 1:658:A:TYR:HB3  | 1:658:A:TYR:HA   | 14       | 0.21          |
| (1,101) | 1:658:A:TYR:HB3  | 1:658:A:TYR:HA   | 19       | 0.21          |
| (1,70)  | 1:641:A:GLU:HB3  | 1:638:A:ASP:HA   | 20       | 0.21          |
| (3,31)  | 1:664:A:LEU:HD11 | 2:542:B:PHE:HD1  | 20       | 0.2           |
| (3,31)  | 1:664:A:LEU:HD11 | 2:542:B:PHE:HD2  | 20       | 0.2           |
| (3,31)  | 1:664:A:LEU:HD12 | 2:542:B:PHE:HD1  | 20       | 0.2           |
| (3,31)  | 1:664:A:LEU:HD12 | 2:542:B:PHE:HD2  | 20       | 0.2           |
| (3,31)  | 1:664:A:LEU:HD13 | 2:542:B:PHE:HD1  | 20       | 0.2           |
| (3,31)  | 1:664:A:LEU:HD13 | 2:542:B:PHE:HD2  | 20       | 0.2           |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB2  | 13       | 0.2           |
| (3,29)  | 1:664:A:LEU:HA   | 2:539:B:ASP:HB3  | 13       | 0.2           |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD1  | 20       | 0.2           |
| (3,27)  | 1:660:A:ILE:HD11 | 2:534:B:PHE:HD2  | 20       | 0.2           |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD1  | 20       | 0.2           |
| (3,27)  | 1:660:A:ILE:HD12 | 2:534:B:PHE:HD2  | 20       | 0.2           |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD1  | 20       | 0.2           |
| (3,27)  | 1:660:A:ILE:HD13 | 2:534:B:PHE:HD2  | 20       | 0.2           |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD21 | 1        | 0.2           |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD22 | 1        | 0.2           |
| (3,13)  | 1:625:A:MET:HA   | 2:545:B:LEU:HD23 | 1        | 0.2           |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD11 | 16       | 0.2           |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD12 | 16       | 0.2           |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD13 | 16       | 0.2           |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD11 | 16       | 0.2           |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD12 | 16       | 0.2           |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD13 | 16       | 0.2           |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD21 | 16       | 0.2           |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD22 | 16       | 0.2           |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD23 | 16       | 0.2           |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD21 | 16       | 0.2           |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD22 | 16       | 0.2           |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD23 | 16       | 0.2           |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 14       | 0.2           |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 14       | 0.2           |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 14       | 0.2           |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 14       | 0.2           |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 14       | 0.2           |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 14       | 0.2           |
| (2,245) | 2:537:B:ILE:H    | 2:537:B:ILE:HG12 | 1        | 0.2           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,242) | 2:539:B:ASP:H    | 2:539:B:ASP:HB2  | 20       | 0.2           |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 11       | 0.2           |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 17       | 0.2           |
| (2,196) | 2:541:B:ASP:H    | 2:541:B:ASP:HB3  | 11       | 0.2           |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 1        | 0.2           |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 3        | 0.2           |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 8        | 0.2           |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 11       | 0.2           |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 3        | 0.2           |
| (2,127) | 2:542:B:PHE:HA   | 2:545:B:LEU:HB3  | 19       | 0.2           |
| (2,121) | 2:540:B:MET:HA   | 2:540:B:MET:HG2  | 7        | 0.2           |
| (2,121) | 2:540:B:MET:HA   | 2:540:B:MET:HG2  | 11       | 0.2           |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 9        | 0.2           |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 9        | 0.2           |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 9        | 0.2           |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 15       | 0.2           |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 15       | 0.2           |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 15       | 0.2           |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 2        | 0.2           |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 5        | 0.2           |
| (2,93)  | 2:534:B:PHE:HD1  | 2:534:B:PHE:HB3  | 10       | 0.2           |
| (2,93)  | 2:534:B:PHE:HD2  | 2:534:B:PHE:HB3  | 10       | 0.2           |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 2        | 0.2           |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 5        | 0.2           |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 14       | 0.2           |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 14       | 0.2           |
| (1,999) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 14       | 0.2           |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 14       | 0.2           |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 14       | 0.2           |
| (1,998) | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 14       | 0.2           |
| (1,993) | 1:619:A:ALA:HB1  | 1:612:A:PHE:HZ   | 18       | 0.2           |
| (1,993) | 1:619:A:ALA:HB2  | 1:612:A:PHE:HZ   | 18       | 0.2           |
| (1,993) | 1:619:A:ALA:HB3  | 1:612:A:PHE:HZ   | 18       | 0.2           |
| (1,982) | 1:607:A:LEU:H    | 1:606:A:LYS:HB2  | 17       | 0.2           |
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 10       | 0.2           |
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 10       | 0.2           |
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 20       | 0.2           |
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 20       | 0.2           |
| (1,966) | 1:661:A:GLN:H    | 1:660:A:ILE:HG22 | 6        | 0.2           |
| (1,966) | 1:661:A:GLN:H    | 1:660:A:ILE:HG22 | 13       | 0.2           |
| (1,952) | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 7        | 0.2           |
| (1,951) | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 17       | 0.2           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,950) | 1:671:A:ARG:H    | 1:671:A:ARG:HB2  | 14       | 0.2           |
| (1,944) | 1:666:A:GLU:H    | 1:666:A:GLU:HG2  | 2        | 0.2           |
| (1,944) | 1:666:A:GLU:H    | 1:666:A:GLU:HG2  | 10       | 0.2           |
| (1,866) | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 2        | 0.2           |
| (1,866) | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 14       | 0.2           |
| (1,866) | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 20       | 0.2           |
| (1,805) | 1:621:A:LYS:H    | 1:621:A:LYS:HG3  | 20       | 0.2           |
| (1,785) | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 6        | 0.2           |
| (1,785) | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 15       | 0.2           |
| (1,723) | 1:609:A:GLN:H    | 1:608:A:VAL:HG13 | 5        | 0.2           |
| (1,723) | 1:609:A:GLN:H    | 1:608:A:VAL:HG11 | 11       | 0.2           |
| (1,695) | 1:641:A:GLU:H    | 1:641:A:GLU:HG2  | 2        | 0.2           |
| (1,688) | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 12       | 0.2           |
| (1,688) | 1:597:A:GLN:HE22 | 1:597:A:GLN:HG2  | 18       | 0.2           |
| (1,677) | 1:643:A:ALA:H    | 1:642:A:SER:HB2  | 11       | 0.2           |
| (1,672) | 1:593:A:GLU:H    | 1:593:A:GLU:HG2  | 16       | 0.2           |
| (1,606) | 1:595:A:VAL:HA   | 1:599:A:LEU:HD22 | 13       | 0.2           |
| (1,592) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HE2  | 12       | 0.2           |
| (1,582) | 1:599:A:LEU:HD23 | 1:599:A:LEU:HD11 | 5        | 0.2           |
| (1,549) | 1:603:A:LEU:HD22 | 1:606:A:LYS:HD2  | 20       | 0.2           |
| (1,529) | 1:649:A:TYR:HB2  | 1:646:A:ARG:HA   | 18       | 0.2           |
| (1,504) | 1:629:A:VAL:HG11 | 1:629:A:VAL:HG23 | 2        | 0.2           |
| (1,504) | 1:629:A:VAL:HG11 | 1:629:A:VAL:HG21 | 7        | 0.2           |
| (1,496) | 1:599:A:LEU:HD11 | 1:603:A:LEU:HD21 | 20       | 0.2           |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD23 | 14       | 0.2           |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 10       | 0.2           |
| (1,443) | 1:625:A:MET:HG2  | 1:625:A:MET:HE1  | 13       | 0.2           |
| (1,435) | 1:653:A:LEU:HD12 | 1:639:A:MET:HE2  | 18       | 0.2           |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 1        | 0.2           |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 15       | 0.2           |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG22 | 15       | 0.2           |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 11       | 0.2           |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 3        | 0.2           |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 6        | 0.2           |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 19       | 0.2           |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 20       | 0.2           |
| (1,366) | 1:639:A:MET:HE1  | 1:653:A:LEU:HD22 | 17       | 0.2           |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 6        | 0.2           |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 11       | 0.2           |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 18       | 0.2           |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 20       | 0.2           |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 4        | 0.2           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 8        | 0.2           |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 9        | 0.2           |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 12       | 0.2           |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 14       | 0.2           |
| (1,272) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB2  | 2        | 0.2           |
| (1,272) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB2  | 13       | 0.2           |
| (1,272) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB2  | 15       | 0.2           |
| (1,272) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB2  | 17       | 0.2           |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 3        | 0.2           |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 7        | 0.2           |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 5        | 0.2           |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 7        | 0.2           |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 16       | 0.2           |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 18       | 0.2           |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 6        | 0.2           |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 18       | 0.2           |
| (1,225) | 1:632:A:ALA:HB2  | 1:604:A:VAL:HG21 | 6        | 0.2           |
| (1,224) | 1:604:A:VAL:HG11 | 1:604:A:VAL:HG23 | 4        | 0.2           |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 6        | 0.2           |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 17       | 0.2           |
| (1,93)  | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE2  | 13       | 0.2           |
| (1,71)  | 1:641:A:GLU:HG2  | 1:638:A:ASP:HA   | 1        | 0.2           |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 2        | 0.2           |
| (1,23)  | 1:653:A:LEU:HB3  | 1:653:A:LEU:HD11 | 12       | 0.2           |
| (1,21)  | 1:664:A:LEU:HD23 | 1:664:A:LEU:HD11 | 13       | 0.2           |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 15       | 0.19          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 15       | 0.19          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 15       | 0.19          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 15       | 0.19          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 15       | 0.19          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 15       | 0.19          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 15       | 0.19          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 15       | 0.19          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 15       | 0.19          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 4        | 0.19          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 4        | 0.19          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 4        | 0.19          |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 4        | 0.19          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 4        | 0.19          |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 4        | 0.19          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 6        | 0.19          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 6        | 0.19          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 6        | 0.19          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 6        | 0.19          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 6        | 0.19          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 6        | 0.19          |
| (2,276) | 2:547:B:SER:H    | 2:546:B:LEU:HG   | 20       | 0.19          |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 15       | 0.19          |
| (2,185) | 2:540:B:MET:HG3  | 2:540:B:MET:HB3  | 10       | 0.19          |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 6        | 0.19          |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 7        | 0.19          |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 13       | 0.19          |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 19       | 0.19          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 1        | 0.19          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD21 | 6        | 0.19          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD22 | 6        | 0.19          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD23 | 6        | 0.19          |
| (2,143) | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 7        | 0.19          |
| (2,143) | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 7        | 0.19          |
| (2,143) | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 7        | 0.19          |
| (2,143) | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 9        | 0.19          |
| (2,143) | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 9        | 0.19          |
| (2,143) | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 9        | 0.19          |
| (2,121) | 2:540:B:MET:HA   | 2:540:B:MET:HG2  | 5        | 0.19          |
| (2,121) | 2:540:B:MET:HA   | 2:540:B:MET:HG2  | 15       | 0.19          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD11 | 15       | 0.19          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD12 | 15       | 0.19          |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD13 | 15       | 0.19          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD11 | 15       | 0.19          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD12 | 15       | 0.19          |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD13 | 15       | 0.19          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 11       | 0.19          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 15       | 0.19          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 16       | 0.19          |
| (2,76)  | 2:542:B:PHE:HA   | 2:542:B:PHE:HD1  | 20       | 0.19          |
| (2,76)  | 2:542:B:PHE:HA   | 2:542:B:PHE:HD2  | 20       | 0.19          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 11       | 0.19          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 15       | 0.19          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 16       | 0.19          |
| (2,34)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HA   | 19       | 0.19          |
| (2,32)  | 2:549:B:ILE:HA   | 2:549:B:ILE:HG12 | 19       | 0.19          |
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 3        | 0.19          |
| (1,979) | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 3        | 0.19          |
| (1,966) | 1:661:A:GLN:H    | 1:660:A:ILE:HG22 | 7        | 0.19          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,866) | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 1        | 0.19          |
| (1,866) | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 10       | 0.19          |
| (1,866) | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 13       | 0.19          |
| (1,866) | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 15       | 0.19          |
| (1,866) | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 18       | 0.19          |
| (1,787) | 1:616:A:ASP:H    | 1:614:A:THR:HG23 | 20       | 0.19          |
| (1,785) | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 3        | 0.19          |
| (1,696) | 1:614:A:THR:H    | 1:614:A:THR:HB   | 17       | 0.19          |
| (1,658) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG22 | 1        | 0.19          |
| (1,592) | 1:634:A:LYS:HG2  | 1:634:A:LYS:HE2  | 8        | 0.19          |
| (1,583) | 1:603:A:LEU:HD12 | 1:599:A:LEU:HD11 | 20       | 0.19          |
| (1,582) | 1:599:A:LEU:HD21 | 1:599:A:LEU:HD12 | 8        | 0.19          |
| (1,504) | 1:629:A:VAL:HG13 | 1:629:A:VAL:HG23 | 9        | 0.19          |
| (1,504) | 1:629:A:VAL:HG11 | 1:629:A:VAL:HG22 | 10       | 0.19          |
| (1,504) | 1:629:A:VAL:HG11 | 1:629:A:VAL:HG23 | 16       | 0.19          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 6        | 0.19          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 9        | 0.19          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 6        | 0.19          |
| (1,399) | 1:607:A:LEU:HA   | 1:610:A:ALA:HB1  | 11       | 0.19          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 15       | 0.19          |
| (1,378) | 1:615:A:PRO:HB2  | 1:615:A:PRO:HA   | 18       | 0.19          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 1        | 0.19          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 2        | 0.19          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 3        | 0.19          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 9        | 0.19          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 10       | 0.19          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 14       | 0.19          |
| (1,319) | 1:652:A:LEU:HB2  | 1:652:A:LEU:HA   | 17       | 0.19          |
| (1,302) | 1:614:A:THR:HG23 | 1:617:A:PRO:HA   | 20       | 0.19          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG13 | 10       | 0.19          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 3        | 0.19          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 5        | 0.19          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 16       | 0.19          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 4        | 0.19          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 18       | 0.19          |
| (1,272) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB2  | 19       | 0.19          |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 8        | 0.19          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 12       | 0.19          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 9        | 0.19          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 11       | 0.19          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 14       | 0.19          |
| (1,230) | 1:604:A:VAL:HG21 | 1:604:A:VAL:HA   | 1        | 0.19          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,225) | 1:632:A:ALA:HB2  | 1:604:A:VAL:HG21 | 2        | 0.19          |
| (1,224) | 1:604:A:VAL:HG11 | 1:604:A:VAL:HG21 | 20       | 0.19          |
| (1,223) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HA   | 1        | 0.19          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 7        | 0.19          |
| (1,188) | 1:621:A:LYS:HD2  | 1:621:A:LYS:HE2  | 12       | 0.19          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 10       | 0.19          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 14       | 0.19          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 19       | 0.19          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB1  | 3        | 0.19          |
| (1,173) | 1:651:A:HIS:HA   | 1:651:A:HIS:HB2  | 9        | 0.19          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 19       | 0.19          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 19       | 0.19          |
| (1,97)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HD3  | 14       | 0.19          |
| (1,93)  | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE2  | 9        | 0.19          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 13       | 0.19          |
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD11 | 11       | 0.19          |
| (1,3)   | 1:639:A:MET:HG3  | 1:639:A:MET:HE3  | 3        | 0.19          |
| (1,2)   | 1:639:A:MET:HG2  | 1:639:A:MET:HE2  | 3        | 0.19          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD11 | 2        | 0.18          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD12 | 2        | 0.18          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD13 | 2        | 0.18          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD11 | 2        | 0.18          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD12 | 2        | 0.18          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD13 | 2        | 0.18          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD11 | 15       | 0.18          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD12 | 15       | 0.18          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD13 | 15       | 0.18          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD11 | 15       | 0.18          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD12 | 15       | 0.18          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD13 | 15       | 0.18          |
| (2,273) | 2:545:B:LEU:H    | 2:545:B:LEU:HD11 | 7        | 0.18          |
| (2,256) | 2:538:B:ALA:H    | 2:537:B:ILE:HG22 | 2        | 0.18          |
| (2,245) | 2:537:B:ILE:H    | 2:537:B:ILE:HG12 | 7        | 0.18          |
| (2,245) | 2:537:B:ILE:H    | 2:537:B:ILE:HG12 | 13       | 0.18          |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 2        | 0.18          |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 5        | 0.18          |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 16       | 0.18          |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 19       | 0.18          |
| (2,169) | 2:544:B:ALA:HA   | 2:547:B:SER:HB3  | 7        | 0.18          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 12       | 0.18          |
| (2,151) | 2:546:B:LEU:HB2  | 2:547:B:SER:HA   | 19       | 0.18          |
| (2,143) | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 1        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,143)  | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 1        | 0.18          |
| (2,143)  | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 1        | 0.18          |
| (2,143)  | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 13       | 0.18          |
| (2,143)  | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 13       | 0.18          |
| (2,143)  | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 13       | 0.18          |
| (2,143)  | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 19       | 0.18          |
| (2,143)  | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 19       | 0.18          |
| (2,143)  | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 19       | 0.18          |
| (2,127)  | 2:542:B:PHE:HA   | 2:545:B:LEU:HB3  | 1        | 0.18          |
| (2,125)  | 2:545:B:LEU:HB2  | 2:542:B:PHE:HA   | 13       | 0.18          |
| (2,108)  | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 6        | 0.18          |
| (2,108)  | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 8        | 0.18          |
| (2,108)  | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 14       | 0.18          |
| (2,76)   | 2:542:B:PHE:HA   | 2:542:B:PHE:HD1  | 16       | 0.18          |
| (2,76)   | 2:542:B:PHE:HA   | 2:542:B:PHE:HD2  | 16       | 0.18          |
| (2,72)   | 2:537:B:ILE:HB   | 2:534:B:PHE:HD1  | 13       | 0.18          |
| (2,72)   | 2:537:B:ILE:HB   | 2:534:B:PHE:HD2  | 13       | 0.18          |
| (2,61)   | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 6        | 0.18          |
| (2,61)   | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 8        | 0.18          |
| (2,61)   | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 14       | 0.18          |
| (2,34)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HA   | 7        | 0.18          |
| (2,34)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HA   | 12       | 0.18          |
| (2,32)   | 2:549:B:ILE:HA   | 2:549:B:ILE:HG12 | 7        | 0.18          |
| (2,32)   | 2:549:B:ILE:HA   | 2:549:B:ILE:HG12 | 12       | 0.18          |
| (1,1007) | 1:640:A:TYR:HA   | 1:591:A:TRP:HZ2  | 18       | 0.18          |
| (1,982)  | 1:607:A:LEU:H    | 1:606:A:LYS:HB2  | 14       | 0.18          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 16       | 0.18          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 16       | 0.18          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD1  | 19       | 0.18          |
| (1,979)  | 1:612:A:PHE:H    | 1:612:A:PHE:HD2  | 19       | 0.18          |
| (1,966)  | 1:661:A:GLN:H    | 1:660:A:ILE:HG23 | 5        | 0.18          |
| (1,912)  | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 20       | 0.18          |
| (1,888)  | 1:651:A:HIS:H    | 1:651:A:HIS:HB3  | 9        | 0.18          |
| (1,866)  | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 12       | 0.18          |
| (1,778)  | 1:611:A:ILE:H    | 1:611:A:ILE:HG12 | 2        | 0.18          |
| (1,694)  | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 3        | 0.18          |
| (1,694)  | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 7        | 0.18          |
| (1,694)  | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 12       | 0.18          |
| (1,694)  | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 13       | 0.18          |
| (1,694)  | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 19       | 0.18          |
| (1,657)  | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE1  | 10       | 0.18          |
| (1,657)  | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE2  | 10       | 0.18          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,650) | 1:648:A:GLU:HG3  | 1:648:A:GLU:HA   | 19       | 0.18          |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD12 | 6        | 0.18          |
| (1,627) | 1:612:A:PHE:HB2  | 1:628:A:LEU:HD23 | 3        | 0.18          |
| (1,582) | 1:599:A:LEU:HD21 | 1:599:A:LEU:HD12 | 2        | 0.18          |
| (1,582) | 1:599:A:LEU:HD22 | 1:599:A:LEU:HD13 | 14       | 0.18          |
| (1,549) | 1:603:A:LEU:HD23 | 1:606:A:LYS:HD2  | 8        | 0.18          |
| (1,513) | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 7        | 0.18          |
| (1,513) | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 12       | 0.18          |
| (1,504) | 1:629:A:VAL:HG11 | 1:629:A:VAL:HG22 | 6        | 0.18          |
| (1,504) | 1:629:A:VAL:HG11 | 1:629:A:VAL:HG21 | 13       | 0.18          |
| (1,504) | 1:629:A:VAL:HG13 | 1:629:A:VAL:HG23 | 15       | 0.18          |
| (1,475) | 1:599:A:LEU:HB2  | 1:595:A:VAL:HG11 | 12       | 0.18          |
| (1,472) | 1:662:A:LYS:HA   | 1:665:A:GLU:HB2  | 17       | 0.18          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD22 | 16       | 0.18          |
| (1,464) | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 14       | 0.18          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 14       | 0.18          |
| (1,459) | 1:607:A:LEU:HB2  | 1:607:A:LEU:HD21 | 10       | 0.18          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 5        | 0.18          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 16       | 0.18          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 17       | 0.18          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 19       | 0.18          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG23 | 8        | 0.18          |
| (1,412) | 1:630:A:ALA:HB1  | 1:627:A:ASN:HA   | 2        | 0.18          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 17       | 0.18          |
| (1,399) | 1:607:A:LEU:HA   | 1:610:A:ALA:HB1  | 17       | 0.18          |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG11 | 3        | 0.18          |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG13 | 11       | 0.18          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG13 | 17       | 0.18          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG12 | 12       | 0.18          |
| (1,290) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 14       | 0.18          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 7        | 0.18          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 20       | 0.18          |
| (1,242) | 1:668:A:ARG:HB2  | 1:665:A:GLU:HA   | 16       | 0.18          |
| (1,225) | 1:632:A:ALA:HB3  | 1:604:A:VAL:HG21 | 5        | 0.18          |
| (1,224) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HG23 | 13       | 0.18          |
| (1,223) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HA   | 2        | 0.18          |
| (1,223) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HA   | 11       | 0.18          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 4        | 0.18          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 14       | 0.18          |
| (1,187) | 1:621:A:LYS:HE2  | 1:621:A:LYS:HG3  | 2        | 0.18          |
| (1,155) | 1:605:A:HIS:HB2  | 1:602:A:HIS:HA   | 17       | 0.18          |
| (1,151) | 1:602:A:HIS:HB3  | 1:602:A:HIS:HD2  | 14       | 0.18          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,140) | 1:643:A:ALA:HB2  | 1:640:A:TYR:HA   | 7        | 0.18          |
| (1,91)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HE2  | 1        | 0.18          |
| (1,90)  | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE3  | 19       | 0.18          |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 12       | 0.18          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 8        | 0.18          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 17       | 0.18          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 20       | 0.18          |
| (1,54)  | 1:613:A:PRO:HG3  | 1:612:A:PHE:HA   | 4        | 0.18          |
| (1,21)  | 1:664:A:LEU:HD21 | 1:664:A:LEU:HD12 | 16       | 0.18          |
| (1,6)   | 1:608:A:VAL:HG13 | 1:625:A:MET:HE3  | 9        | 0.18          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD11 | 9        | 0.17          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD12 | 9        | 0.17          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD13 | 9        | 0.17          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD11 | 9        | 0.17          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD12 | 9        | 0.17          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD13 | 9        | 0.17          |
| (2,252) | 2:535:B:SER:H    | 2:534:B:PHE:HD1  | 8        | 0.17          |
| (2,250) | 2:534:B:PHE:H    | 2:534:B:PHE:HD1  | 2        | 0.17          |
| (2,245) | 2:537:B:ILE:H    | 2:537:B:ILE:HG12 | 6        | 0.17          |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 8        | 0.17          |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 8        | 0.17          |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 11       | 0.17          |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 14       | 0.17          |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 2        | 0.17          |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 14       | 0.17          |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 15       | 0.17          |
| (2,127) | 2:542:B:PHE:HA   | 2:545:B:LEU:HB3  | 5        | 0.17          |
| (2,121) | 2:540:B:MET:HA   | 2:540:B:MET:HG2  | 2        | 0.17          |
| (2,121) | 2:540:B:MET:HA   | 2:540:B:MET:HG2  | 4        | 0.17          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 3        | 0.17          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 4        | 0.17          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 9        | 0.17          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 10       | 0.17          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 17       | 0.17          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 18       | 0.17          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 3        | 0.17          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 4        | 0.17          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 9        | 0.17          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 10       | 0.17          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 17       | 0.17          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 18       | 0.17          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 6        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 6        | 0.17          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 6        | 0.17          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 12       | 0.17          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 12       | 0.17          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 12       | 0.17          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 18       | 0.17          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 18       | 0.17          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 18       | 0.17          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 19       | 0.17          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 19       | 0.17          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 19       | 0.17          |
| (2,34)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HA   | 6        | 0.17          |
| (2,32)   | 2:549:B:ILE:HA   | 2:549:B:ILE:HG12 | 6        | 0.17          |
| (1,1007) | 1:640:A:TYR:HA   | 1:591:A:TRP:HZ2  | 20       | 0.17          |
| (1,999)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 15       | 0.17          |
| (1,999)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 15       | 0.17          |
| (1,999)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 15       | 0.17          |
| (1,998)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD11 | 15       | 0.17          |
| (1,998)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD12 | 15       | 0.17          |
| (1,998)  | 1:612:A:PHE:HB3  | 1:628:A:LEU:HD13 | 15       | 0.17          |
| (1,993)  | 1:619:A:ALA:HB1  | 1:612:A:PHE:HZ   | 13       | 0.17          |
| (1,993)  | 1:619:A:ALA:HB2  | 1:612:A:PHE:HZ   | 13       | 0.17          |
| (1,993)  | 1:619:A:ALA:HB3  | 1:612:A:PHE:HZ   | 13       | 0.17          |
| (1,987)  | 1:603:A:LEU:H    | 1:603:A:LEU:HD23 | 1        | 0.17          |
| (1,984)  | 1:607:A:LEU:H    | 1:607:A:LEU:HB3  | 6        | 0.17          |
| (1,982)  | 1:607:A:LEU:H    | 1:606:A:LYS:HB2  | 3        | 0.17          |
| (1,955)  | 1:672:A:LEU:H    | 1:671:A:ARG:H    | 14       | 0.17          |
| (1,952)  | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 10       | 0.17          |
| (1,949)  | 1:671:A:ARG:H    | 1:671:A:ARG:HB3  | 1        | 0.17          |
| (1,949)  | 1:671:A:ARG:H    | 1:671:A:ARG:HB3  | 4        | 0.17          |
| (1,949)  | 1:671:A:ARG:H    | 1:671:A:ARG:HB3  | 11       | 0.17          |
| (1,915)  | 1:657:A:ILE:H    | 1:657:A:ILE:HD11 | 11       | 0.17          |
| (1,915)  | 1:657:A:ILE:H    | 1:657:A:ILE:HD11 | 18       | 0.17          |
| (1,912)  | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 6        | 0.17          |
| (1,912)  | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 7        | 0.17          |
| (1,912)  | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 8        | 0.17          |
| (1,912)  | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 16       | 0.17          |
| (1,866)  | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 7        | 0.17          |
| (1,805)  | 1:621:A:LYS:H    | 1:621:A:LYS:HG3  | 10       | 0.17          |
| (1,785)  | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 5        | 0.17          |
| (1,785)  | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 8        | 0.17          |
| (1,785)  | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 9        | 0.17          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,785) | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 12       | 0.17          |
| (1,785) | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 13       | 0.17          |
| (1,778) | 1:611:A:ILE:H    | 1:611:A:ILE:HG12 | 17       | 0.17          |
| (1,717) | 1:610:A:ALA:H    | 1:657:A:ILE:HD13 | 2        | 0.17          |
| (1,696) | 1:614:A:THR:H    | 1:614:A:THR:HB   | 5        | 0.17          |
| (1,696) | 1:614:A:THR:H    | 1:614:A:THR:HB   | 13       | 0.17          |
| (1,696) | 1:614:A:THR:H    | 1:614:A:THR:HB   | 19       | 0.17          |
| (1,694) | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 1        | 0.17          |
| (1,694) | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 2        | 0.17          |
| (1,694) | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 4        | 0.17          |
| (1,694) | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 5        | 0.17          |
| (1,694) | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 10       | 0.17          |
| (1,694) | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 14       | 0.17          |
| (1,694) | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 15       | 0.17          |
| (1,694) | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 18       | 0.17          |
| (1,677) | 1:643:A:ALA:H    | 1:642:A:SER:HB2  | 1        | 0.17          |
| (1,672) | 1:593:A:GLU:H    | 1:593:A:GLU:HG2  | 7        | 0.17          |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD12 | 2        | 0.17          |
| (1,644) | 1:608:A:VAL:HA   | 1:611:A:ILE:HD13 | 8        | 0.17          |
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD11 | 7        | 0.17          |
| (1,582) | 1:599:A:LEU:HD23 | 1:599:A:LEU:HD11 | 4        | 0.17          |
| (1,582) | 1:599:A:LEU:HD22 | 1:599:A:LEU:HD11 | 7        | 0.17          |
| (1,574) | 1:657:A:ILE:HD13 | 1:657:A:ILE:HG23 | 15       | 0.17          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 6        | 0.17          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 17       | 0.17          |
| (1,513) | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 19       | 0.17          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 2        | 0.17          |
| (1,504) | 1:629:A:VAL:HG13 | 1:629:A:VAL:HG23 | 5        | 0.17          |
| (1,504) | 1:629:A:VAL:HG13 | 1:629:A:VAL:HG22 | 17       | 0.17          |
| (1,504) | 1:629:A:VAL:HG12 | 1:629:A:VAL:HG22 | 19       | 0.17          |
| (1,498) | 1:639:A:MET:HG2  | 1:652:A:LEU:HD21 | 10       | 0.17          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD23 | 8        | 0.17          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD22 | 9        | 0.17          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD21 | 11       | 0.17          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD23 | 18       | 0.17          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 3        | 0.17          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 4        | 0.17          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 5        | 0.17          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 7        | 0.17          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 8        | 0.17          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 9        | 0.17          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 11       | 0.17          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 18       | 0.17          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 19       | 0.17          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 20       | 0.17          |
| (1,419) | 1:629:A:VAL:HG23 | 1:626:A:GLU:HA   | 3        | 0.17          |
| (1,412) | 1:630:A:ALA:HB1  | 1:627:A:ASN:HA   | 4        | 0.17          |
| (1,412) | 1:630:A:ALA:HB3  | 1:627:A:ASN:HA   | 14       | 0.17          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 9        | 0.17          |
| (1,399) | 1:607:A:LEU:HA   | 1:610:A:ALA:HB3  | 2        | 0.17          |
| (1,399) | 1:607:A:LEU:HA   | 1:610:A:ALA:HB1  | 8        | 0.17          |
| (1,349) | 1:610:A:ALA:HB2  | 1:657:A:ILE:HD11 | 20       | 0.17          |
| (1,337) | 1:611:A:ILE:HD13 | 1:611:A:ILE:HB   | 13       | 0.17          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG12 | 1        | 0.17          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG12 | 3        | 0.17          |
| (1,291) | 1:633:A:LYS:HD2  | 1:633:A:LYS:HG2  | 1        | 0.17          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 17       | 0.17          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 19       | 0.17          |
| (1,270) | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 19       | 0.17          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 4        | 0.17          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 19       | 0.17          |
| (1,224) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HG23 | 19       | 0.17          |
| (1,207) | 1:632:A:ALA:HA   | 1:607:A:LEU:HD11 | 16       | 0.17          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 5        | 0.17          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 18       | 0.17          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 1        | 0.17          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 1        | 0.17          |
| (1,90)  | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE3  | 10       | 0.17          |
| (1,77)  | 1:672:A:LEU:HD11 | 1:672:A:LEU:HB3  | 9        | 0.17          |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 18       | 0.17          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 2        | 0.17          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 9        | 0.17          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 16       | 0.17          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 19       | 0.17          |
| (1,54)  | 1:613:A:PRO:HG3  | 1:612:A:PHE:HA   | 3        | 0.17          |
| (1,54)  | 1:613:A:PRO:HG3  | 1:612:A:PHE:HA   | 6        | 0.17          |
| (1,6)   | 1:608:A:VAL:HG13 | 1:625:A:MET:HE2  | 16       | 0.17          |
| (2,264) | 2:541:B:ASP:H    | 2:540:B:MET:HB3  | 3        | 0.16          |
| (2,261) | 2:540:B:MET:H    | 2:539:B:ASP:HB2  | 20       | 0.16          |
| (2,256) | 2:538:B:ALA:H    | 2:537:B:ILE:HG21 | 5        | 0.16          |
| (2,245) | 2:537:B:ILE:H    | 2:537:B:ILE:HG12 | 4        | 0.16          |
| (2,245) | 2:537:B:ILE:H    | 2:537:B:ILE:HG12 | 12       | 0.16          |
| (2,245) | 2:537:B:ILE:H    | 2:537:B:ILE:HG12 | 19       | 0.16          |
| (2,244) | 2:535:B:SER:H    | 2:534:B:PHE:HA   | 6        | 0.16          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 1        | 0.16          |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 12       | 0.16          |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 18       | 0.16          |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 2        | 0.16          |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 3        | 0.16          |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 9        | 0.16          |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 10       | 0.16          |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 5        | 0.16          |
| (2,183) | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 16       | 0.16          |
| (2,181) | 2:540:B:MET:HA   | 2:540:B:MET:HB2  | 13       | 0.16          |
| (2,121) | 2:540:B:MET:HA   | 2:540:B:MET:HG2  | 6        | 0.16          |
| (2,121) | 2:540:B:MET:HA   | 2:540:B:MET:HG2  | 8        | 0.16          |
| (2,121) | 2:540:B:MET:HA   | 2:540:B:MET:HG2  | 12       | 0.16          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 18       | 0.16          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 18       | 0.16          |
| (2,110) | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 18       | 0.16          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 7        | 0.16          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 13       | 0.16          |
| (2,76)  | 2:542:B:PHE:HA   | 2:542:B:PHE:HD1  | 9        | 0.16          |
| (2,76)  | 2:542:B:PHE:HA   | 2:542:B:PHE:HD2  | 9        | 0.16          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD1  | 17       | 0.16          |
| (2,74)  | 2:542:B:PHE:HB3  | 2:542:B:PHE:HD2  | 17       | 0.16          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 7        | 0.16          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 13       | 0.16          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 1        | 0.16          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 1        | 0.16          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 1        | 0.16          |
| (2,34)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HA   | 1        | 0.16          |
| (2,34)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HA   | 5        | 0.16          |
| (2,34)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HA   | 16       | 0.16          |
| (2,32)  | 2:549:B:ILE:HA   | 2:549:B:ILE:HG12 | 1        | 0.16          |
| (2,32)  | 2:549:B:ILE:HA   | 2:549:B:ILE:HG12 | 5        | 0.16          |
| (2,32)  | 2:549:B:ILE:HA   | 2:549:B:ILE:HG12 | 16       | 0.16          |
| (1,973) | 1:655:A:GLU:H    | 1:651:A:HIS:HA   | 2        | 0.16          |
| (1,966) | 1:661:A:GLN:H    | 1:660:A:ILE:HG22 | 8        | 0.16          |
| (1,949) | 1:671:A:ARG:H    | 1:671:A:ARG:HB3  | 17       | 0.16          |
| (1,915) | 1:657:A:ILE:H    | 1:657:A:ILE:HD13 | 4        | 0.16          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 9        | 0.16          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 14       | 0.16          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 16       | 0.16          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 18       | 0.16          |
| (1,866) | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 6        | 0.16          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,853) | 1:635:A:VAL:H    | 1:635:A:VAL:HG11 | 13       | 0.16          |
| (1,785) | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 1        | 0.16          |
| (1,785) | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 2        | 0.16          |
| (1,785) | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 16       | 0.16          |
| (1,778) | 1:611:A:ILE:H    | 1:611:A:ILE:HG12 | 19       | 0.16          |
| (1,763) | 1:605:A:HIS:H    | 1:604:A:VAL:HG11 | 8        | 0.16          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 6        | 0.16          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 9        | 0.16          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 20       | 0.16          |
| (1,723) | 1:609:A:GLN:H    | 1:608:A:VAL:HG11 | 16       | 0.16          |
| (1,695) | 1:641:A:GLU:H    | 1:641:A:GLU:HG2  | 19       | 0.16          |
| (1,689) | 1:670:A:SER:H    | 1:670:A:SER:HB2  | 1        | 0.16          |
| (1,677) | 1:643:A:ALA:H    | 1:642:A:SER:HB2  | 17       | 0.16          |
| (1,672) | 1:593:A:GLU:H    | 1:593:A:GLU:HG2  | 14       | 0.16          |
| (1,582) | 1:599:A:LEU:HD22 | 1:599:A:LEU:HD12 | 13       | 0.16          |
| (1,581) | 1:602:A:HIS:HB3  | 1:599:A:LEU:HA   | 14       | 0.16          |
| (1,540) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD13 | 13       | 0.16          |
| (1,520) | 1:668:A:ARG:HA   | 1:668:A:ARG:HG3  | 14       | 0.16          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 4        | 0.16          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 6        | 0.16          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 7        | 0.16          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 11       | 0.16          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 12       | 0.16          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 14       | 0.16          |
| (1,504) | 1:629:A:VAL:HG11 | 1:629:A:VAL:HG21 | 1        | 0.16          |
| (1,504) | 1:629:A:VAL:HG12 | 1:629:A:VAL:HG22 | 8        | 0.16          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD23 | 10       | 0.16          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD23 | 13       | 0.16          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD21 | 15       | 0.16          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD21 | 20       | 0.16          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 1        | 0.16          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 2        | 0.16          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 6        | 0.16          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 12       | 0.16          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 15       | 0.16          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 16       | 0.16          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 17       | 0.16          |
| (1,460) | 1:656:A:LYS:HB2  | 1:656:A:LYS:HA   | 20       | 0.16          |
| (1,455) | 1:614:A:THR:HB   | 1:614:A:THR:HA   | 7        | 0.16          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 13       | 0.16          |
| (1,416) | 1:658:A:TYR:HA   | 1:657:A:ILE:HG22 | 2        | 0.16          |
| (1,412) | 1:630:A:ALA:HB1  | 1:627:A:ASN:HA   | 10       | 0.16          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,411) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HB2  | 1        | 0.16          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 12       | 0.16          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 16       | 0.16          |
| (1,402) | 1:629:A:VAL:HG12 | 1:630:A:ALA:HA   | 17       | 0.16          |
| (1,392) | 1:635:A:VAL:HG21 | 1:632:A:ALA:HA   | 1        | 0.16          |
| (1,380) | 1:620:A:LEU:HD13 | 1:617:A:PRO:HA   | 5        | 0.16          |
| (1,374) | 1:633:A:LYS:HE2  | 1:629:A:VAL:HG13 | 10       | 0.16          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG12 | 19       | 0.16          |
| (1,333) | 1:657:A:ILE:HA   | 1:657:A:ILE:HG23 | 9        | 0.16          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 17       | 0.16          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE1  | 2        | 0.16          |
| (1,144) | 1:592:A:HIS:HA   | 1:640:A:TYR:HE2  | 2        | 0.16          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE1  | 4        | 0.16          |
| (1,143) | 1:595:A:VAL:HB   | 1:640:A:TYR:HE2  | 4        | 0.16          |
| (1,122) | 1:595:A:VAL:HG22 | 1:649:A:TYR:HE1  | 11       | 0.16          |
| (1,122) | 1:595:A:VAL:HG22 | 1:649:A:TYR:HE2  | 11       | 0.16          |
| (1,97)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HD3  | 15       | 0.16          |
| (1,93)  | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE2  | 17       | 0.16          |
| (1,90)  | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE3  | 18       | 0.16          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 3        | 0.16          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 4        | 0.16          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 6        | 0.16          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 7        | 0.16          |
| (1,54)  | 1:613:A:PRO:HG3  | 1:612:A:PHE:HA   | 7        | 0.16          |
| (1,54)  | 1:613:A:PRO:HG3  | 1:612:A:PHE:HA   | 12       | 0.16          |
| (1,54)  | 1:613:A:PRO:HG3  | 1:612:A:PHE:HA   | 14       | 0.16          |
| (1,23)  | 1:653:A:LEU:HB3  | 1:653:A:LEU:HD12 | 17       | 0.16          |
| (1,21)  | 1:664:A:LEU:HD23 | 1:664:A:LEU:HD13 | 10       | 0.16          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 4        | 0.15          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 4        | 0.15          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 4        | 0.15          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 4        | 0.15          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 4        | 0.15          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 4        | 0.15          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 4        | 0.15          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 4        | 0.15          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 4        | 0.15          |
| (2,245) | 2:537:B:ILE:H    | 2:537:B:ILE:HG12 | 3        | 0.15          |
| (2,245) | 2:537:B:ILE:H    | 2:537:B:ILE:HG12 | 9        | 0.15          |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 10       | 0.15          |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 13       | 0.15          |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 1        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,205)  | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 6        | 0.15          |
| (2,205)  | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 17       | 0.15          |
| (2,205)  | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 18       | 0.15          |
| (2,184)  | 2:540:B:MET:HG3  | 2:540:B:MET:HB2  | 10       | 0.15          |
| (2,183)  | 2:540:B:MET:HG2  | 2:540:B:MET:HB3  | 20       | 0.15          |
| (2,181)  | 2:540:B:MET:HA   | 2:540:B:MET:HB2  | 16       | 0.15          |
| (2,144)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD21 | 18       | 0.15          |
| (2,144)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD22 | 18       | 0.15          |
| (2,144)  | 2:546:B:LEU:HA   | 2:546:B:LEU:HD23 | 18       | 0.15          |
| (2,143)  | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 5        | 0.15          |
| (2,143)  | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 5        | 0.15          |
| (2,143)  | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 5        | 0.15          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD11 | 2        | 0.15          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD12 | 2        | 0.15          |
| (2,110)  | 2:534:B:PHE:HB2  | 2:537:B:ILE:HD13 | 2        | 0.15          |
| (2,76)   | 2:542:B:PHE:HA   | 2:542:B:PHE:HD1  | 8        | 0.15          |
| (2,76)   | 2:542:B:PHE:HA   | 2:542:B:PHE:HD2  | 8        | 0.15          |
| (2,64)   | 2:537:B:ILE:HA   | 2:537:B:ILE:HD11 | 20       | 0.15          |
| (2,64)   | 2:537:B:ILE:HA   | 2:537:B:ILE:HD12 | 20       | 0.15          |
| (2,64)   | 2:537:B:ILE:HA   | 2:537:B:ILE:HD13 | 20       | 0.15          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 11       | 0.15          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 11       | 0.15          |
| (2,42)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 11       | 0.15          |
| (2,34)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HA   | 8        | 0.15          |
| (2,34)   | 2:549:B:ILE:HG12 | 2:549:B:ILE:HA   | 13       | 0.15          |
| (2,32)   | 2:549:B:ILE:HA   | 2:549:B:ILE:HG12 | 8        | 0.15          |
| (2,32)   | 2:549:B:ILE:HA   | 2:549:B:ILE:HG12 | 13       | 0.15          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG11 | 9        | 0.15          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG12 | 9        | 0.15          |
| (1,1006) | 1:607:A:LEU:HD11 | 1:635:A:VAL:HG13 | 9        | 0.15          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG11 | 9        | 0.15          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG12 | 9        | 0.15          |
| (1,1006) | 1:607:A:LEU:HD12 | 1:635:A:VAL:HG13 | 9        | 0.15          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG11 | 9        | 0.15          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG12 | 9        | 0.15          |
| (1,1006) | 1:607:A:LEU:HD13 | 1:635:A:VAL:HG13 | 9        | 0.15          |
| (1,1003) | 1:608:A:VAL:HG11 | 1:632:A:ALA:HB1  | 19       | 0.15          |
| (1,1003) | 1:608:A:VAL:HG11 | 1:632:A:ALA:HB2  | 19       | 0.15          |
| (1,1003) | 1:608:A:VAL:HG11 | 1:632:A:ALA:HB3  | 19       | 0.15          |
| (1,1003) | 1:608:A:VAL:HG12 | 1:632:A:ALA:HB1  | 19       | 0.15          |
| (1,1003) | 1:608:A:VAL:HG12 | 1:632:A:ALA:HB2  | 19       | 0.15          |
| (1,1003) | 1:608:A:VAL:HG12 | 1:632:A:ALA:HB3  | 19       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1003) | 1:608:A:VAL:HG13 | 1:632:A:ALA:HB1  | 19       | 0.15          |
| (1,1003) | 1:608:A:VAL:HG13 | 1:632:A:ALA:HB2  | 19       | 0.15          |
| (1,1003) | 1:608:A:VAL:HG13 | 1:632:A:ALA:HB3  | 19       | 0.15          |
| (1,966)  | 1:661:A:GLN:H    | 1:660:A:ILE:HG23 | 12       | 0.15          |
| (1,952)  | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 2        | 0.15          |
| (1,952)  | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 15       | 0.15          |
| (1,951)  | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 1        | 0.15          |
| (1,912)  | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 3        | 0.15          |
| (1,907)  | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 1        | 0.15          |
| (1,907)  | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 5        | 0.15          |
| (1,907)  | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 7        | 0.15          |
| (1,907)  | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 12       | 0.15          |
| (1,907)  | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 15       | 0.15          |
| (1,903)  | 1:653:A:LEU:H    | 1:653:A:LEU:HD13 | 3        | 0.15          |
| (1,866)  | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 8        | 0.15          |
| (1,845)  | 1:632:A:ALA:H    | 1:631:A:TYR:HD1  | 18       | 0.15          |
| (1,845)  | 1:632:A:ALA:H    | 1:631:A:TYR:HD2  | 18       | 0.15          |
| (1,785)  | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 4        | 0.15          |
| (1,785)  | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 17       | 0.15          |
| (1,764)  | 1:606:A:LYS:H    | 1:602:A:HIS:HA   | 11       | 0.15          |
| (1,749)  | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 13       | 0.15          |
| (1,742)  | 1:599:A:LEU:H    | 1:599:A:LEU:HG   | 9        | 0.15          |
| (1,696)  | 1:614:A:THR:H    | 1:614:A:THR:HB   | 18       | 0.15          |
| (1,694)  | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 8        | 0.15          |
| (1,694)  | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 9        | 0.15          |
| (1,694)  | 1:641:A:GLU:H    | 1:641:A:GLU:HB3  | 17       | 0.15          |
| (1,682)  | 1:642:A:SER:H    | 1:641:A:GLU:HB3  | 6        | 0.15          |
| (1,657)  | 1:595:A:VAL:HG12 | 1:649:A:TYR:HE1  | 3        | 0.15          |
| (1,657)  | 1:595:A:VAL:HG12 | 1:649:A:TYR:HE2  | 3        | 0.15          |
| (1,513)  | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 17       | 0.15          |
| (1,513)  | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 18       | 0.15          |
| (1,506)  | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 3        | 0.15          |
| (1,506)  | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 20       | 0.15          |
| (1,504)  | 1:629:A:VAL:HG11 | 1:629:A:VAL:HG23 | 18       | 0.15          |
| (1,496)  | 1:599:A:LEU:HD12 | 1:603:A:LEU:HD21 | 6        | 0.15          |
| (1,489)  | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 8        | 0.15          |
| (1,489)  | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 14       | 0.15          |
| (1,469)  | 1:635:A:VAL:HA   | 1:635:A:VAL:HG13 | 14       | 0.15          |
| (1,468)  | 1:607:A:LEU:HG   | 1:607:A:LEU:HD23 | 2        | 0.15          |
| (1,459)  | 1:607:A:LEU:HB2  | 1:607:A:LEU:HD21 | 18       | 0.15          |
| (1,459)  | 1:607:A:LEU:HB2  | 1:607:A:LEU:HD23 | 19       | 0.15          |
| (1,455)  | 1:614:A:THR:HB   | 1:614:A:THR:HA   | 1        | 0.15          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,455) | 1:614:A:THR:HB   | 1:614:A:THR:HA   | 2        | 0.15          |
| (1,455) | 1:614:A:THR:HB   | 1:614:A:THR:HA   | 10       | 0.15          |
| (1,455) | 1:614:A:THR:HB   | 1:614:A:THR:HA   | 12       | 0.15          |
| (1,455) | 1:614:A:THR:HB   | 1:614:A:THR:HA   | 15       | 0.15          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 6        | 0.15          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 14       | 0.15          |
| (1,402) | 1:629:A:VAL:HG11 | 1:630:A:ALA:HA   | 14       | 0.15          |
| (1,392) | 1:635:A:VAL:HG21 | 1:632:A:ALA:HA   | 4        | 0.15          |
| (1,354) | 1:660:A:ILE:HD13 | 1:657:A:ILE:HA   | 10       | 0.15          |
| (1,349) | 1:610:A:ALA:HB3  | 1:657:A:ILE:HD12 | 5        | 0.15          |
| (1,337) | 1:611:A:ILE:HD11 | 1:611:A:ILE:HB   | 20       | 0.15          |
| (1,333) | 1:657:A:ILE:HA   | 1:657:A:ILE:HG21 | 2        | 0.15          |
| (1,290) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 2        | 0.15          |
| (1,287) | 1:671:A:ARG:HB2  | 1:671:A:ARG:HD2  | 20       | 0.15          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 6        | 0.15          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 17       | 0.15          |
| (1,246) | 1:659:A:LYS:HE2  | 1:659:A:LYS:HD3  | 1        | 0.15          |
| (1,227) | 1:603:A:LEU:HB3  | 1:604:A:VAL:HG23 | 2        | 0.15          |
| (1,223) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HA   | 20       | 0.15          |
| (1,212) | 1:611:A:ILE:HD11 | 1:607:A:LEU:HD21 | 12       | 0.15          |
| (1,212) | 1:611:A:ILE:HD12 | 1:607:A:LEU:HD21 | 12       | 0.15          |
| (1,212) | 1:611:A:ILE:HD13 | 1:607:A:LEU:HD21 | 12       | 0.15          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 3        | 0.15          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 20       | 0.15          |
| (1,155) | 1:605:A:HIS:HB2  | 1:602:A:HIS:HA   | 7        | 0.15          |
| (1,142) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE1  | 7        | 0.15          |
| (1,142) | 1:595:A:VAL:HG13 | 1:640:A:TYR:HE2  | 7        | 0.15          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD1  | 1        | 0.15          |
| (1,117) | 1:653:A:LEU:HD23 | 1:650:A:TYR:HD2  | 1        | 0.15          |
| (1,117) | 1:653:A:LEU:HD21 | 1:650:A:TYR:HD1  | 17       | 0.15          |
| (1,117) | 1:653:A:LEU:HD21 | 1:650:A:TYR:HD2  | 17       | 0.15          |
| (1,90)  | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE3  | 2        | 0.15          |
| (1,90)  | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE3  | 5        | 0.15          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 11       | 0.15          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 12       | 0.15          |
| (1,57)  | 1:613:A:PRO:HD2  | 1:613:A:PRO:HA   | 14       | 0.15          |
| (3,32)  | 1:664:A:LEU:HD11 | 2:542:B:PHE:HE1  | 2        | 0.14          |
| (3,32)  | 1:664:A:LEU:HD11 | 2:542:B:PHE:HE2  | 2        | 0.14          |
| (3,32)  | 1:664:A:LEU:HD12 | 2:542:B:PHE:HE1  | 2        | 0.14          |
| (3,32)  | 1:664:A:LEU:HD12 | 2:542:B:PHE:HE2  | 2        | 0.14          |
| (3,32)  | 1:664:A:LEU:HD13 | 2:542:B:PHE:HE1  | 2        | 0.14          |
| (3,32)  | 1:664:A:LEU:HD13 | 2:542:B:PHE:HE2  | 2        | 0.14          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,21)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD1  | 10       | 0.14          |
| (3,21)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD2  | 10       | 0.14          |
| (3,21)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD1  | 10       | 0.14          |
| (3,21)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD2  | 10       | 0.14          |
| (3,21)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD1  | 10       | 0.14          |
| (3,21)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD2  | 10       | 0.14          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 1        | 0.14          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 1        | 0.14          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD1  | 15       | 0.14          |
| (3,3)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HD2  | 15       | 0.14          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD1  | 15       | 0.14          |
| (3,3)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HD2  | 15       | 0.14          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD1  | 15       | 0.14          |
| (3,3)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HD2  | 15       | 0.14          |
| (2,264) | 2:541:B:ASP:H    | 2:540:B:MET:HB3  | 17       | 0.14          |
| (2,245) | 2:537:B:ILE:H    | 2:537:B:ILE:HG12 | 8        | 0.14          |
| (2,244) | 2:535:B:SER:H    | 2:534:B:PHE:HA   | 11       | 0.14          |
| (2,203) | 2:535:B:SER:H    | 2:535:B:SER:HB2  | 7        | 0.14          |
| (2,181) | 2:540:B:MET:HA   | 2:540:B:MET:HB2  | 19       | 0.14          |
| (2,143) | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 18       | 0.14          |
| (2,143) | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 18       | 0.14          |
| (2,143) | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 18       | 0.14          |
| (2,143) | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 20       | 0.14          |
| (2,143) | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 20       | 0.14          |
| (2,143) | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 20       | 0.14          |
| (2,121) | 2:540:B:MET:HA   | 2:540:B:MET:HG2  | 3        | 0.14          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 1        | 0.14          |
| (2,77)  | 2:547:B:SER:HB3  | 2:544:B:ALA:HA   | 14       | 0.14          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 1        | 0.14          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 2        | 0.14          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 2        | 0.14          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 2        | 0.14          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 9        | 0.14          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 9        | 0.14          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 9        | 0.14          |
| (1,984) | 1:607:A:LEU:H    | 1:607:A:LEU:HB3  | 4        | 0.14          |
| (1,973) | 1:655:A:GLU:H    | 1:651:A:HIS:HA   | 6        | 0.14          |
| (1,973) | 1:655:A:GLU:H    | 1:651:A:HIS:HA   | 20       | 0.14          |
| (1,966) | 1:661:A:GLN:H    | 1:660:A:ILE:HG22 | 11       | 0.14          |
| (1,966) | 1:661:A:GLN:H    | 1:660:A:ILE:HG21 | 17       | 0.14          |
| (1,952) | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 13       | 0.14          |
| (1,952) | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 20       | 0.14          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,940) | 1:664:A:LEU:H    | 1:663:A:GLU:HB3  | 17       | 0.14          |
| (1,937) | 1:663:A:GLU:H    | 1:662:A:LYS:HB2  | 14       | 0.14          |
| (1,912) | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 11       | 0.14          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 2        | 0.14          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 13       | 0.14          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 17       | 0.14          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 20       | 0.14          |
| (1,903) | 1:653:A:LEU:H    | 1:653:A:LEU:HD12 | 16       | 0.14          |
| (1,764) | 1:606:A:LYS:H    | 1:602:A:HIS:HA   | 18       | 0.14          |
| (1,764) | 1:606:A:LYS:H    | 1:602:A:HIS:HA   | 19       | 0.14          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 4        | 0.14          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 5        | 0.14          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 11       | 0.14          |
| (1,724) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HD2  | 1        | 0.14          |
| (1,695) | 1:641:A:GLU:H    | 1:641:A:GLU:HG2  | 13       | 0.14          |
| (1,689) | 1:670:A:SER:H    | 1:670:A:SER:HB2  | 4        | 0.14          |
| (1,672) | 1:593:A:GLU:H    | 1:593:A:GLU:HG2  | 11       | 0.14          |
| (1,574) | 1:657:A:ILE:HD13 | 1:657:A:ILE:HG21 | 14       | 0.14          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 11       | 0.14          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD22 | 17       | 0.14          |
| (1,464) | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 2        | 0.14          |
| (1,464) | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 17       | 0.14          |
| (1,451) | 1:665:A:GLU:HB3  | 1:665:A:GLU:HA   | 1        | 0.14          |
| (1,444) | 1:625:A:MET:HG3  | 1:625:A:MET:HE2  | 5        | 0.14          |
| (1,444) | 1:625:A:MET:HG3  | 1:625:A:MET:HE3  | 19       | 0.14          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 4        | 0.14          |
| (1,428) | 1:661:A:GLN:HA   | 1:661:A:GLN:HG3  | 8        | 0.14          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 7        | 0.14          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 19       | 0.14          |
| (1,399) | 1:607:A:LEU:HA   | 1:610:A:ALA:HB1  | 1        | 0.14          |
| (1,363) | 1:654:A:ALA:HA   | 1:657:A:ILE:HG23 | 2        | 0.14          |
| (1,333) | 1:657:A:ILE:HA   | 1:657:A:ILE:HG23 | 4        | 0.14          |
| (1,295) | 1:633:A:LYS:HA   | 1:604:A:VAL:HG13 | 7        | 0.14          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 1        | 0.14          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 8        | 0.14          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 13       | 0.14          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 14       | 0.14          |
| (1,262) | 1:629:A:VAL:HA   | 1:632:A:ALA:HB3  | 12       | 0.14          |
| (1,224) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HG21 | 8        | 0.14          |
| (1,223) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HA   | 5        | 0.14          |
| (1,223) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HA   | 6        | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 1        | 0.14          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 2        | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 3        | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 4        | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 6        | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 7        | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 8        | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 9        | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 10       | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 11       | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 13       | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 14       | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 16       | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 17       | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 18       | 0.14          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 19       | 0.14          |
| (1,173) | 1:651:A:HIS:HA   | 1:651:A:HIS:HB2  | 11       | 0.14          |
| (1,173) | 1:651:A:HIS:HA   | 1:651:A:HIS:HB2  | 13       | 0.14          |
| (1,171) | 1:608:A:VAL:HB   | 1:605:A:HIS:HD2  | 14       | 0.14          |
| (1,155) | 1:605:A:HIS:HB2  | 1:602:A:HIS:HA   | 5        | 0.14          |
| (1,155) | 1:605:A:HIS:HB2  | 1:602:A:HIS:HA   | 9        | 0.14          |
| (1,155) | 1:605:A:HIS:HB2  | 1:602:A:HIS:HA   | 18       | 0.14          |
| (1,77)  | 1:672:A:LEU:HD13 | 1:672:A:LEU:HB3  | 12       | 0.14          |
| (3,20)  | 1:628:A:LEU:HB2  | 2:538:B:ALA:HA   | 17       | 0.13          |
| (3,20)  | 1:628:A:LEU:HB3  | 2:538:B:ALA:HA   | 17       | 0.13          |
| (2,264) | 2:541:B:ASP:H    | 2:540:B:MET:HB3  | 8        | 0.13          |
| (2,244) | 2:535:B:SER:H    | 2:534:B:PHE:HA   | 13       | 0.13          |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 4        | 0.13          |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 15       | 0.13          |
| (2,181) | 2:540:B:MET:HA   | 2:540:B:MET:HB2  | 9        | 0.13          |
| (2,127) | 2:542:B:PHE:HA   | 2:545:B:LEU:HB3  | 2        | 0.13          |
| (2,121) | 2:540:B:MET:HA   | 2:540:B:MET:HG2  | 1        | 0.13          |
| (2,118) | 2:540:B:MET:HG2  | 2:540:B:MET:HA   | 20       | 0.13          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 12       | 0.13          |
| (2,76)  | 2:542:B:PHE:HA   | 2:542:B:PHE:HD1  | 14       | 0.13          |
| (2,76)  | 2:542:B:PHE:HA   | 2:542:B:PHE:HD2  | 14       | 0.13          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 12       | 0.13          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 5        | 0.13          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 5        | 0.13          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 5        | 0.13          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 8        | 0.13          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 8        | 0.13          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 8        | 0.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 10       | 0.13          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 10       | 0.13          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 10       | 0.13          |
| (2,34)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HA   | 14       | 0.13          |
| (2,32)  | 2:549:B:ILE:HA   | 2:549:B:ILE:HG12 | 14       | 0.13          |
| (1,993) | 1:619:A:ALA:HB1  | 1:612:A:PHE:HZ   | 12       | 0.13          |
| (1,993) | 1:619:A:ALA:HB2  | 1:612:A:PHE:HZ   | 12       | 0.13          |
| (1,993) | 1:619:A:ALA:HB3  | 1:612:A:PHE:HZ   | 12       | 0.13          |
| (1,982) | 1:607:A:LEU:H    | 1:606:A:LYS:HB2  | 18       | 0.13          |
| (1,966) | 1:661:A:GLN:H    | 1:660:A:ILE:HG21 | 18       | 0.13          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 7        | 0.13          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 10       | 0.13          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 11       | 0.13          |
| (1,915) | 1:657:A:ILE:H    | 1:657:A:ILE:HD12 | 12       | 0.13          |
| (1,912) | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 9        | 0.13          |
| (1,912) | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 15       | 0.13          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 19       | 0.13          |
| (1,894) | 1:652:A:LEU:H    | 1:652:A:LEU:HD13 | 7        | 0.13          |
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 5        | 0.13          |
| (1,785) | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 10       | 0.13          |
| (1,785) | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 11       | 0.13          |
| (1,785) | 1:616:A:ASP:H    | 1:615:A:PRO:HB3  | 14       | 0.13          |
| (1,764) | 1:606:A:LYS:H    | 1:602:A:HIS:HA   | 17       | 0.13          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 3        | 0.13          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 8        | 0.13          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 10       | 0.13          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 16       | 0.13          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 17       | 0.13          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 18       | 0.13          |
| (1,723) | 1:609:A:GLN:H    | 1:608:A:VAL:HG12 | 12       | 0.13          |
| (1,723) | 1:609:A:GLN:H    | 1:608:A:VAL:HG12 | 19       | 0.13          |
| (1,677) | 1:643:A:ALA:H    | 1:642:A:SER:HB2  | 18       | 0.13          |
| (1,677) | 1:643:A:ALA:H    | 1:642:A:SER:HB2  | 19       | 0.13          |
| (1,672) | 1:593:A:GLU:H    | 1:593:A:GLU:HG2  | 2        | 0.13          |
| (1,672) | 1:593:A:GLU:H    | 1:593:A:GLU:HG2  | 4        | 0.13          |
| (1,670) | 1:620:A:LEU:H    | 1:620:A:LEU:HD13 | 18       | 0.13          |
| (1,657) | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE1  | 6        | 0.13          |
| (1,657) | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE2  | 6        | 0.13          |
| (1,657) | 1:595:A:VAL:HG12 | 1:649:A:TYR:HE1  | 20       | 0.13          |
| (1,657) | 1:595:A:VAL:HG12 | 1:649:A:TYR:HE2  | 20       | 0.13          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 5        | 0.13          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 9        | 0.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 15       | 0.13          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 18       | 0.13          |
| (1,489) | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 3        | 0.13          |
| (1,489) | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 5        | 0.13          |
| (1,489) | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 9        | 0.13          |
| (1,468) | 1:607:A:LEU:HG   | 1:607:A:LEU:HD22 | 19       | 0.13          |
| (1,464) | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 3        | 0.13          |
| (1,464) | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 4        | 0.13          |
| (1,464) | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 10       | 0.13          |
| (1,412) | 1:630:A:ALA:HB1  | 1:627:A:ASN:HA   | 9        | 0.13          |
| (1,412) | 1:630:A:ALA:HB3  | 1:627:A:ASN:HA   | 11       | 0.13          |
| (1,402) | 1:629:A:VAL:HG13 | 1:630:A:ALA:HA   | 13       | 0.13          |
| (1,375) | 1:633:A:LYS:HD2  | 1:629:A:VAL:HG13 | 10       | 0.13          |
| (1,355) | 1:593:A:GLU:HA   | 1:593:A:GLU:HG2  | 15       | 0.13          |
| (1,349) | 1:610:A:ALA:HB1  | 1:657:A:ILE:HD13 | 9        | 0.13          |
| (1,333) | 1:657:A:ILE:HA   | 1:657:A:ILE:HG21 | 1        | 0.13          |
| (1,333) | 1:657:A:ILE:HA   | 1:657:A:ILE:HG22 | 3        | 0.13          |
| (1,333) | 1:657:A:ILE:HA   | 1:657:A:ILE:HG21 | 15       | 0.13          |
| (1,300) | 1:617:A:PRO:HA   | 1:617:A:PRO:HB2  | 1        | 0.13          |
| (1,300) | 1:617:A:PRO:HA   | 1:617:A:PRO:HB2  | 2        | 0.13          |
| (1,300) | 1:617:A:PRO:HA   | 1:617:A:PRO:HB2  | 9        | 0.13          |
| (1,300) | 1:617:A:PRO:HA   | 1:617:A:PRO:HB2  | 10       | 0.13          |
| (1,300) | 1:617:A:PRO:HA   | 1:617:A:PRO:HB2  | 12       | 0.13          |
| (1,300) | 1:617:A:PRO:HA   | 1:617:A:PRO:HB2  | 15       | 0.13          |
| (1,300) | 1:617:A:PRO:HA   | 1:617:A:PRO:HB2  | 16       | 0.13          |
| (1,300) | 1:617:A:PRO:HA   | 1:617:A:PRO:HB2  | 17       | 0.13          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 3        | 0.13          |
| (1,265) | 1:667:A:LYS:HA   | 1:667:A:LYS:HB3  | 9        | 0.13          |
| (1,224) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HG22 | 5        | 0.13          |
| (1,224) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HG22 | 7        | 0.13          |
| (1,223) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HA   | 9        | 0.13          |
| (1,223) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HA   | 13       | 0.13          |
| (1,209) | 1:607:A:LEU:HA   | 1:607:A:LEU:HD23 | 17       | 0.13          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 12       | 0.13          |
| (1,173) | 1:651:A:HIS:HA   | 1:651:A:HIS:HB2  | 17       | 0.13          |
| (1,167) | 1:605:A:HIS:HA   | 1:605:A:HIS:HD2  | 1        | 0.13          |
| (1,155) | 1:605:A:HIS:HB2  | 1:602:A:HIS:HA   | 15       | 0.13          |
| (1,122) | 1:595:A:VAL:HG23 | 1:649:A:TYR:HE1  | 13       | 0.13          |
| (1,122) | 1:595:A:VAL:HG23 | 1:649:A:TYR:HE2  | 13       | 0.13          |
| (1,122) | 1:595:A:VAL:HG22 | 1:649:A:TYR:HE1  | 19       | 0.13          |
| (1,122) | 1:595:A:VAL:HG22 | 1:649:A:TYR:HE2  | 19       | 0.13          |
| (1,97)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HD3  | 5        | 0.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,91)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HE2  | 11       | 0.13          |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 3        | 0.13          |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 8        | 0.13          |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 15       | 0.13          |
| (1,54)  | 1:613:A:PRO:HG3  | 1:612:A:PHE:HA   | 9        | 0.13          |
| (1,54)  | 1:613:A:PRO:HG3  | 1:612:A:PHE:HA   | 19       | 0.13          |
| (3,21)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD1  | 12       | 0.12          |
| (3,21)  | 1:628:A:LEU:HD11 | 2:534:B:PHE:HD2  | 12       | 0.12          |
| (3,21)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD1  | 12       | 0.12          |
| (3,21)  | 1:628:A:LEU:HD12 | 2:534:B:PHE:HD2  | 12       | 0.12          |
| (3,21)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD1  | 12       | 0.12          |
| (3,21)  | 1:628:A:LEU:HD13 | 2:534:B:PHE:HD2  | 12       | 0.12          |
| (3,18)  | 1:627:A:ASN:HB2  | 2:537:B:ILE:HG21 | 11       | 0.12          |
| (3,18)  | 1:627:A:ASN:HB2  | 2:537:B:ILE:HG22 | 11       | 0.12          |
| (3,18)  | 1:627:A:ASN:HB2  | 2:537:B:ILE:HG23 | 11       | 0.12          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD21 | 11       | 0.12          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD22 | 11       | 0.12          |
| (3,5)   | 1:612:A:PHE:HB2  | 2:545:B:LEU:HD23 | 11       | 0.12          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD21 | 11       | 0.12          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD22 | 11       | 0.12          |
| (3,5)   | 1:612:A:PHE:HB3  | 2:545:B:LEU:HD23 | 11       | 0.12          |
| (2,245) | 2:537:B:ILE:H    | 2:537:B:ILE:HG12 | 17       | 0.12          |
| (2,245) | 2:537:B:ILE:H    | 2:537:B:ILE:HG12 | 18       | 0.12          |
| (2,244) | 2:535:B:SER:H    | 2:534:B:PHE:HA   | 3        | 0.12          |
| (2,244) | 2:535:B:SER:H    | 2:534:B:PHE:HA   | 4        | 0.12          |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 5        | 0.12          |
| (2,203) | 2:535:B:SER:H    | 2:535:B:SER:HB2  | 13       | 0.12          |
| (2,203) | 2:535:B:SER:H    | 2:535:B:SER:HB2  | 16       | 0.12          |
| (2,184) | 2:540:B:MET:HG3  | 2:540:B:MET:HB2  | 9        | 0.12          |
| (2,181) | 2:540:B:MET:HA   | 2:540:B:MET:HB2  | 14       | 0.12          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD21 | 13       | 0.12          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD22 | 13       | 0.12          |
| (2,144) | 2:546:B:LEU:HA   | 2:546:B:LEU:HD23 | 13       | 0.12          |
| (2,136) | 2:543:B:SER:HA   | 2:546:B:LEU:HB3  | 3        | 0.12          |
| (2,108) | 2:537:B:ILE:HG13 | 2:537:B:ILE:HB   | 19       | 0.12          |
| (2,62)  | 2:537:B:ILE:HA   | 2:537:B:ILE:HG13 | 16       | 0.12          |
| (2,61)  | 2:537:B:ILE:HB   | 2:537:B:ILE:HG13 | 19       | 0.12          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 13       | 0.12          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 13       | 0.12          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 13       | 0.12          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 14       | 0.12          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 14       | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 14       | 0.12          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 16       | 0.12          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 16       | 0.12          |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 16       | 0.12          |
| (1,973) | 1:655:A:GLU:H    | 1:651:A:HIS:HA   | 1        | 0.12          |
| (1,973) | 1:655:A:GLU:H    | 1:651:A:HIS:HA   | 16       | 0.12          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 3        | 0.12          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 4        | 0.12          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 5        | 0.12          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 6        | 0.12          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 16       | 0.12          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 18       | 0.12          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 20       | 0.12          |
| (1,952) | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 4        | 0.12          |
| (1,951) | 1:671:A:ARG:H    | 1:671:A:ARG:HG2  | 4        | 0.12          |
| (1,912) | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 12       | 0.12          |
| (1,912) | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 13       | 0.12          |
| (1,912) | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 17       | 0.12          |
| (1,912) | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 18       | 0.12          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 4        | 0.12          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 8        | 0.12          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 11       | 0.12          |
| (1,894) | 1:652:A:LEU:H    | 1:652:A:LEU:HD13 | 12       | 0.12          |
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 1        | 0.12          |
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 6        | 0.12          |
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 20       | 0.12          |
| (1,764) | 1:606:A:LYS:H    | 1:602:A:HIS:HA   | 15       | 0.12          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 1        | 0.12          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 7        | 0.12          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 12       | 0.12          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 19       | 0.12          |
| (1,732) | 1:594:A:HIS:H    | 1:593:A:GLU:HB3  | 12       | 0.12          |
| (1,725) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HG3  | 8        | 0.12          |
| (1,724) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HD2  | 12       | 0.12          |
| (1,689) | 1:670:A:SER:H    | 1:670:A:SER:HB2  | 17       | 0.12          |
| (1,677) | 1:643:A:ALA:H    | 1:642:A:SER:HB2  | 12       | 0.12          |
| (1,672) | 1:593:A:GLU:H    | 1:593:A:GLU:HG2  | 5        | 0.12          |
| (1,657) | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE1  | 8        | 0.12          |
| (1,657) | 1:595:A:VAL:HG11 | 1:649:A:TYR:HE2  | 8        | 0.12          |
| (1,595) | 1:635:A:VAL:HG22 | 1:635:A:VAL:HG12 | 13       | 0.12          |
| (1,537) | 1:653:A:LEU:HD23 | 1:653:A:LEU:HD13 | 7        | 0.12          |
| (1,513) | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 2        | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,513) | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 8        | 0.12          |
| (1,513) | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 14       | 0.12          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 1        | 0.12          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 8        | 0.12          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 10       | 0.12          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 13       | 0.12          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 16       | 0.12          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 17       | 0.12          |
| (1,506) | 1:615:A:PRO:HB3  | 1:615:A:PRO:HG2  | 19       | 0.12          |
| (1,503) | 1:625:A:MET:HG2  | 1:629:A:VAL:HG23 | 6        | 0.12          |
| (1,489) | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 4        | 0.12          |
| (1,489) | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 17       | 0.12          |
| (1,489) | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 19       | 0.12          |
| (1,464) | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 5        | 0.12          |
| (1,464) | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 16       | 0.12          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB1  | 2        | 0.12          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB2  | 4        | 0.12          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB1  | 6        | 0.12          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB1  | 7        | 0.12          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB3  | 8        | 0.12          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB1  | 9        | 0.12          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB1  | 11       | 0.12          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB1  | 12       | 0.12          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB2  | 13       | 0.12          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB1  | 16       | 0.12          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB2  | 18       | 0.12          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB2  | 19       | 0.12          |
| (1,444) | 1:625:A:MET:HG3  | 1:625:A:MET:HE1  | 1        | 0.12          |
| (1,415) | 1:620:A:LEU:HD21 | 1:625:A:MET:HG2  | 3        | 0.12          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 1        | 0.12          |
| (1,409) | 1:592:A:HIS:H    | 1:591:A:TRP:HB2  | 3        | 0.12          |
| (1,390) | 1:628:A:LEU:HD13 | 1:628:A:LEU:HB2  | 6        | 0.12          |
| (1,373) | 1:626:A:GLU:HA   | 1:629:A:VAL:HG11 | 4        | 0.12          |
| (1,355) | 1:593:A:GLU:HA   | 1:593:A:GLU:HG2  | 20       | 0.12          |
| (1,290) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 8        | 0.12          |
| (1,272) | 1:641:A:GLU:HG2  | 1:641:A:GLU:HB2  | 20       | 0.12          |
| (1,271) | 1:667:A:LYS:HE2  | 1:667:A:LYS:HD2  | 1        | 0.12          |
| (1,270) | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 11       | 0.12          |
| (1,270) | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 20       | 0.12          |
| (1,245) | 1:659:A:LYS:HB3  | 1:659:A:LYS:HA   | 5        | 0.12          |
| (1,245) | 1:659:A:LYS:HB3  | 1:659:A:LYS:HA   | 8        | 0.12          |
| (1,245) | 1:659:A:LYS:HB3  | 1:659:A:LYS:HA   | 15       | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,245) | 1:659:A:LYS:HB3  | 1:659:A:LYS:HA   | 20       | 0.12          |
| (1,230) | 1:604:A:VAL:HG23 | 1:604:A:VAL:HA   | 14       | 0.12          |
| (1,224) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HG23 | 14       | 0.12          |
| (1,221) | 1:607:A:LEU:HB3  | 1:604:A:VAL:HA   | 13       | 0.12          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 16       | 0.12          |
| (1,181) | 1:621:A:LYS:HB2  | 1:621:A:LYS:HA   | 15       | 0.12          |
| (1,140) | 1:643:A:ALA:HB2  | 1:640:A:TYR:HA   | 4        | 0.12          |
| (1,97)  | 1:662:A:LYS:HB2  | 1:662:A:LYS:HD3  | 6        | 0.12          |
| (1,91)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HE2  | 7        | 0.12          |
| (1,90)  | 1:662:A:LYS:HG3  | 1:662:A:LYS:HE3  | 15       | 0.12          |
| (1,78)  | 1:672:A:LEU:HB2  | 1:672:A:LEU:HD12 | 6        | 0.12          |
| (1,78)  | 1:672:A:LEU:HB2  | 1:672:A:LEU:HD12 | 8        | 0.12          |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 7        | 0.12          |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 17       | 0.12          |
| (1,54)  | 1:613:A:PRO:HG3  | 1:612:A:PHE:HA   | 8        | 0.12          |
| (1,54)  | 1:613:A:PRO:HG3  | 1:612:A:PHE:HA   | 11       | 0.12          |
| (1,54)  | 1:613:A:PRO:HG3  | 1:612:A:PHE:HA   | 16       | 0.12          |
| (1,23)  | 1:653:A:LEU:HB3  | 1:653:A:LEU:HD11 | 5        | 0.12          |
| (3,18)  | 1:627:A:ASN:HB2  | 2:537:B:ILE:HG21 | 19       | 0.11          |
| (3,18)  | 1:627:A:ASN:HB2  | 2:537:B:ILE:HG22 | 19       | 0.11          |
| (3,18)  | 1:627:A:ASN:HB2  | 2:537:B:ILE:HG23 | 19       | 0.11          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD11 | 11       | 0.11          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD12 | 11       | 0.11          |
| (3,10)  | 1:624:A:ARG:HB2  | 2:545:B:LEU:HD13 | 11       | 0.11          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD11 | 11       | 0.11          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD12 | 11       | 0.11          |
| (3,10)  | 1:624:A:ARG:HB3  | 2:545:B:LEU:HD13 | 11       | 0.11          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD21 | 5        | 0.11          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD22 | 5        | 0.11          |
| (3,9)   | 1:619:A:ALA:HB1  | 2:545:B:LEU:HD23 | 5        | 0.11          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD21 | 5        | 0.11          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD22 | 5        | 0.11          |
| (3,9)   | 1:619:A:ALA:HB2  | 2:545:B:LEU:HD23 | 5        | 0.11          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD21 | 5        | 0.11          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD22 | 5        | 0.11          |
| (3,9)   | 1:619:A:ALA:HB3  | 2:545:B:LEU:HD23 | 5        | 0.11          |
| (2,269) | 2:543:B:SER:H    | 2:542:B:PHE:HB3  | 3        | 0.11          |
| (2,264) | 2:541:B:ASP:H    | 2:540:B:MET:HB3  | 18       | 0.11          |
| (2,261) | 2:540:B:MET:H    | 2:539:B:ASP:HB2  | 13       | 0.11          |
| (2,256) | 2:538:B:ALA:H    | 2:537:B:ILE:HG22 | 10       | 0.11          |
| (2,244) | 2:535:B:SER:H    | 2:534:B:PHE:HA   | 2        | 0.11          |
| (2,244) | 2:535:B:SER:H    | 2:534:B:PHE:HA   | 10       | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,244) | 2:535:B:SER:H    | 2:534:B:PHE:HA   | 20       | 0.11          |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 9        | 0.11          |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 14       | 0.11          |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 16       | 0.11          |
| (2,203) | 2:535:B:SER:H    | 2:535:B:SER:HB2  | 4        | 0.11          |
| (2,203) | 2:535:B:SER:H    | 2:535:B:SER:HB2  | 11       | 0.11          |
| (2,203) | 2:535:B:SER:H    | 2:535:B:SER:HB2  | 12       | 0.11          |
| (2,203) | 2:535:B:SER:H    | 2:535:B:SER:HB2  | 14       | 0.11          |
| (2,203) | 2:535:B:SER:H    | 2:535:B:SER:HB2  | 15       | 0.11          |
| (2,184) | 2:540:B:MET:HG3  | 2:540:B:MET:HB2  | 17       | 0.11          |
| (2,184) | 2:540:B:MET:HG3  | 2:540:B:MET:HB2  | 18       | 0.11          |
| (2,171) | 2:549:B:ILE:HG13 | 2:549:B:ILE:HB   | 15       | 0.11          |
| (2,143) | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 3        | 0.11          |
| (2,143) | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 3        | 0.11          |
| (2,143) | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 3        | 0.11          |
| (2,137) | 2:543:B:SER:HA   | 2:546:B:LEU:HB2  | 18       | 0.11          |
| (2,127) | 2:542:B:PHE:HA   | 2:545:B:LEU:HB3  | 10       | 0.11          |
| (2,86)  | 2:533:B:ASP:HB2  | 2:533:B:ASP:HA   | 9        | 0.11          |
| (2,86)  | 2:533:B:ASP:HB2  | 2:533:B:ASP:HA   | 10       | 0.11          |
| (2,86)  | 2:533:B:ASP:HB2  | 2:533:B:ASP:HA   | 18       | 0.11          |
| (2,76)  | 2:542:B:PHE:HA   | 2:542:B:PHE:HD1  | 6        | 0.11          |
| (2,76)  | 2:542:B:PHE:HA   | 2:542:B:PHE:HD2  | 6        | 0.11          |
| (1,984) | 1:607:A:LEU:H    | 1:607:A:LEU:HB3  | 5        | 0.11          |
| (1,982) | 1:607:A:LEU:H    | 1:606:A:LYS:HB2  | 1        | 0.11          |
| (1,982) | 1:607:A:LEU:H    | 1:606:A:LYS:HB2  | 7        | 0.11          |
| (1,966) | 1:661:A:GLN:H    | 1:660:A:ILE:HG23 | 3        | 0.11          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 1        | 0.11          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 9        | 0.11          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 14       | 0.11          |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 17       | 0.11          |
| (1,952) | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 16       | 0.11          |
| (1,952) | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 18       | 0.11          |
| (1,952) | 1:672:A:LEU:H    | 1:671:A:ARG:HA   | 19       | 0.11          |
| (1,912) | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 1        | 0.11          |
| (1,912) | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 4        | 0.11          |
| (1,912) | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 10       | 0.11          |
| (1,912) | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 14       | 0.11          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 3        | 0.11          |
| (1,907) | 1:661:A:GLN:H    | 1:661:A:GLN:HB3  | 6        | 0.11          |
| (1,881) | 1:648:A:GLU:H    | 1:643:A:ALA:HB3  | 17       | 0.11          |
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 2        | 0.11          |
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 3        | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 9        | 0.11          |
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 15       | 0.11          |
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 19       | 0.11          |
| (1,866) | 1:639:A:MET:H    | 1:638:A:ASP:HB3  | 17       | 0.11          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD1  | 8        | 0.11          |
| (1,845) | 1:632:A:ALA:H    | 1:631:A:TYR:HD2  | 8        | 0.11          |
| (1,843) | 1:632:A:ALA:H    | 1:631:A:TYR:HB2  | 6        | 0.11          |
| (1,778) | 1:611:A:ILE:H    | 1:611:A:ILE:HG12 | 15       | 0.11          |
| (1,778) | 1:611:A:ILE:H    | 1:611:A:ILE:HG12 | 18       | 0.11          |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 2        | 0.11          |
| (1,732) | 1:594:A:HIS:H    | 1:593:A:GLU:HB3  | 9        | 0.11          |
| (1,689) | 1:670:A:SER:H    | 1:670:A:SER:HB2  | 5        | 0.11          |
| (1,689) | 1:670:A:SER:H    | 1:670:A:SER:HB2  | 10       | 0.11          |
| (1,689) | 1:670:A:SER:H    | 1:670:A:SER:HB2  | 15       | 0.11          |
| (1,642) | 1:603:A:LEU:HB2  | 1:653:A:LEU:HD13 | 8        | 0.11          |
| (1,574) | 1:657:A:ILE:HD13 | 1:657:A:ILE:HG22 | 18       | 0.11          |
| (1,572) | 1:654:A:ALA:HB3  | 1:657:A:ILE:HD13 | 6        | 0.11          |
| (1,557) | 1:629:A:VAL:HG12 | 1:629:A:VAL:HA   | 1        | 0.11          |
| (1,540) | 1:653:A:LEU:HA   | 1:653:A:LEU:HD13 | 10       | 0.11          |
| (1,537) | 1:653:A:LEU:HD23 | 1:653:A:LEU:HD13 | 8        | 0.11          |
| (1,526) | 1:646:A:ARG:HG2  | 1:646:A:ARG:HD3  | 6        | 0.11          |
| (1,526) | 1:646:A:ARG:HG2  | 1:646:A:ARG:HD3  | 18       | 0.11          |
| (1,514) | 1:669:A:ARG:HG2  | 1:669:A:ARG:HD2  | 13       | 0.11          |
| (1,513) | 1:669:A:ARG:HD2  | 1:669:A:ARG:HB2  | 3        | 0.11          |
| (1,500) | 1:648:A:GLU:HG3  | 1:652:A:LEU:HD22 | 10       | 0.11          |
| (1,489) | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 6        | 0.11          |
| (1,489) | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 10       | 0.11          |
| (1,489) | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 15       | 0.11          |
| (1,489) | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 18       | 0.11          |
| (1,489) | 1:670:A:SER:HB2  | 1:670:A:SER:HA   | 20       | 0.11          |
| (1,464) | 1:589:A:LYS:HG3  | 1:589:A:LYS:HE2  | 8        | 0.11          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB1  | 3        | 0.11          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB2  | 5        | 0.11          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB2  | 10       | 0.11          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB3  | 14       | 0.11          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB1  | 15       | 0.11          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB1  | 17       | 0.11          |
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB1  | 20       | 0.11          |
| (1,444) | 1:625:A:MET:HG3  | 1:625:A:MET:HE3  | 17       | 0.11          |
| (1,412) | 1:630:A:ALA:HB3  | 1:627:A:ASN:HA   | 12       | 0.11          |
| (1,412) | 1:630:A:ALA:HB2  | 1:627:A:ASN:HA   | 15       | 0.11          |
| (1,392) | 1:635:A:VAL:HG21 | 1:632:A:ALA:HA   | 6        | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,364) | 1:648:A:GLU:HA   | 1:651:A:HIS:HB2  | 15       | 0.11          |
| (1,364) | 1:648:A:GLU:HA   | 1:651:A:HIS:HB2  | 16       | 0.11          |
| (1,349) | 1:610:A:ALA:HB2  | 1:657:A:ILE:HD12 | 17       | 0.11          |
| (1,337) | 1:611:A:ILE:HD13 | 1:611:A:ILE:HB   | 7        | 0.11          |
| (1,337) | 1:611:A:ILE:HD12 | 1:611:A:ILE:HB   | 16       | 0.11          |
| (1,333) | 1:657:A:ILE:HA   | 1:657:A:ILE:HG22 | 5        | 0.11          |
| (1,333) | 1:657:A:ILE:HA   | 1:657:A:ILE:HG22 | 14       | 0.11          |
| (1,333) | 1:657:A:ILE:HA   | 1:657:A:ILE:HG23 | 20       | 0.11          |
| (1,290) | 1:671:A:ARG:HG2  | 1:671:A:ARG:HD2  | 6        | 0.11          |
| (1,262) | 1:629:A:VAL:HA   | 1:632:A:ALA:HB3  | 4        | 0.11          |
| (1,253) | 1:659:A:LYS:HB3  | 1:659:A:LYS:HG2  | 2        | 0.11          |
| (1,245) | 1:659:A:LYS:HB3  | 1:659:A:LYS:HA   | 1        | 0.11          |
| (1,245) | 1:659:A:LYS:HB3  | 1:659:A:LYS:HA   | 4        | 0.11          |
| (1,245) | 1:659:A:LYS:HB3  | 1:659:A:LYS:HA   | 7        | 0.11          |
| (1,245) | 1:659:A:LYS:HB3  | 1:659:A:LYS:HA   | 11       | 0.11          |
| (1,245) | 1:659:A:LYS:HB3  | 1:659:A:LYS:HA   | 14       | 0.11          |
| (1,223) | 1:604:A:VAL:HG11 | 1:604:A:VAL:HA   | 16       | 0.11          |
| (1,219) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD23 | 9        | 0.11          |
| (1,216) | 1:607:A:LEU:HB2  | 1:607:A:LEU:HA   | 6        | 0.11          |
| (1,214) | 1:607:A:LEU:HB3  | 1:607:A:LEU:HD11 | 1        | 0.11          |
| (1,204) | 1:620:A:LEU:HB3  | 1:620:A:LEU:HD22 | 10       | 0.11          |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 17       | 0.11          |
| (1,176) | 1:651:A:HIS:HD2  | 1:654:A:ALA:HB3  | 2        | 0.11          |
| (1,125) | 1:603:A:LEU:HD21 | 1:650:A:TYR:HE1  | 11       | 0.11          |
| (1,125) | 1:603:A:LEU:HD21 | 1:650:A:TYR:HE2  | 11       | 0.11          |
| (1,89)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HE3  | 14       | 0.11          |
| (1,89)  | 1:662:A:LYS:HG2  | 1:662:A:LYS:HE3  | 16       | 0.11          |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 10       | 0.11          |
| (1,54)  | 1:613:A:PRO:HG3  | 1:612:A:PHE:HA   | 2        | 0.11          |
| (1,24)  | 1:650:A:TYR:HA   | 1:653:A:LEU:HD12 | 10       | 0.11          |
| (1,3)   | 1:639:A:MET:HG3  | 1:639:A:MET:HE1  | 20       | 0.11          |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE1  | 12       | 0.1           |
| (3,4)   | 1:611:A:ILE:HG21 | 2:542:B:PHE:HE2  | 12       | 0.1           |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE1  | 12       | 0.1           |
| (3,4)   | 1:611:A:ILE:HG22 | 2:542:B:PHE:HE2  | 12       | 0.1           |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE1  | 12       | 0.1           |
| (3,4)   | 1:611:A:ILE:HG23 | 2:542:B:PHE:HE2  | 12       | 0.1           |
| (2,248) | 2:537:B:ILE:H    | 2:536:B:SER:HB2  | 17       | 0.1           |
| (2,244) | 2:535:B:SER:H    | 2:534:B:PHE:HA   | 5        | 0.1           |
| (2,244) | 2:535:B:SER:H    | 2:534:B:PHE:HA   | 8        | 0.1           |
| (2,244) | 2:535:B:SER:H    | 2:534:B:PHE:HA   | 12       | 0.1           |
| (2,232) | 2:547:B:SER:H    | 2:546:B:LEU:HA   | 2        | 0.1           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,232) | 2:547:B:SER:H    | 2:546:B:LEU:HA   | 3        | 0.1           |
| (2,232) | 2:547:B:SER:H    | 2:546:B:LEU:HA   | 15       | 0.1           |
| (2,213) | 2:540:B:MET:H    | 2:539:B:ASP:HA   | 19       | 0.1           |
| (2,205) | 2:545:B:LEU:H    | 2:545:B:LEU:HB3  | 12       | 0.1           |
| (2,203) | 2:535:B:SER:H    | 2:535:B:SER:HB2  | 3        | 0.1           |
| (2,203) | 2:535:B:SER:H    | 2:535:B:SER:HB2  | 6        | 0.1           |
| (2,143) | 2:546:B:LEU:HD11 | 2:546:B:LEU:HB2  | 6        | 0.1           |
| (2,143) | 2:546:B:LEU:HD12 | 2:546:B:LEU:HB2  | 6        | 0.1           |
| (2,143) | 2:546:B:LEU:HD13 | 2:546:B:LEU:HB2  | 6        | 0.1           |
| (2,118) | 2:540:B:MET:HG2  | 2:540:B:MET:HA   | 7        | 0.1           |
| (2,118) | 2:540:B:MET:HG2  | 2:540:B:MET:HA   | 11       | 0.1           |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD11 | 19       | 0.1           |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD12 | 19       | 0.1           |
| (2,111) | 2:534:B:PHE:HE1  | 2:537:B:ILE:HD13 | 19       | 0.1           |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD11 | 19       | 0.1           |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD12 | 19       | 0.1           |
| (2,111) | 2:534:B:PHE:HE2  | 2:537:B:ILE:HD13 | 19       | 0.1           |
| (2,76)  | 2:542:B:PHE:HA   | 2:542:B:PHE:HD1  | 13       | 0.1           |
| (2,76)  | 2:542:B:PHE:HA   | 2:542:B:PHE:HD2  | 13       | 0.1           |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG21 | 7        | 0.1           |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG22 | 7        | 0.1           |
| (2,42)  | 2:549:B:ILE:HG12 | 2:549:B:ILE:HG23 | 7        | 0.1           |
| (1,973) | 1:655:A:GLU:H    | 1:651:A:HIS:HA   | 7        | 0.1           |
| (1,973) | 1:655:A:GLU:H    | 1:651:A:HIS:HA   | 8        | 0.1           |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 2        | 0.1           |
| (1,963) | 1:620:A:LEU:H    | 1:620:A:LEU:HB3  | 13       | 0.1           |
| (1,928) | 1:661:A:GLN:HE22 | 1:661:A:GLN:HG3  | 19       | 0.1           |
| (1,915) | 1:657:A:ILE:H    | 1:657:A:ILE:HD11 | 19       | 0.1           |
| (1,912) | 1:657:A:ILE:H    | 1:655:A:GLU:HA   | 19       | 0.1           |
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 8        | 0.1           |
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 10       | 0.1           |
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 17       | 0.1           |
| (1,874) | 1:644:A:ASN:HD22 | 1:644:A:ASN:HB3  | 18       | 0.1           |
| (1,778) | 1:611:A:ILE:H    | 1:611:A:ILE:HG12 | 16       | 0.1           |
| (1,749) | 1:602:A:HIS:H    | 1:602:A:HIS:HB3  | 15       | 0.1           |
| (1,725) | 1:591:A:TRP:HE1  | 1:589:A:LYS:HG3  | 11       | 0.1           |
| (1,723) | 1:609:A:GLN:H    | 1:608:A:VAL:HG13 | 15       | 0.1           |
| (1,695) | 1:641:A:GLU:H    | 1:641:A:GLU:HG2  | 15       | 0.1           |
| (1,677) | 1:643:A:ALA:H    | 1:642:A:SER:HB2  | 20       | 0.1           |
| (1,526) | 1:646:A:ARG:HG2  | 1:646:A:ARG:HD3  | 12       | 0.1           |
| (1,526) | 1:646:A:ARG:HG2  | 1:646:A:ARG:HD3  | 13       | 0.1           |
| (1,526) | 1:646:A:ARG:HG2  | 1:646:A:ARG:HD3  | 20       | 0.1           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,463) | 1:618:A:ALA:HA   | 1:618:A:ALA:HB3  | 1        | 0.1           |
| (1,337) | 1:611:A:ILE:HD11 | 1:611:A:ILE:HB   | 14       | 0.1           |
| (1,333) | 1:657:A:ILE:HA   | 1:657:A:ILE:HG21 | 17       | 0.1           |
| (1,270) | 1:667:A:LYS:HB2  | 1:667:A:LYS:HD2  | 18       | 0.1           |
| (1,262) | 1:629:A:VAL:HA   | 1:632:A:ALA:HB1  | 7        | 0.1           |
| (1,262) | 1:629:A:VAL:HA   | 1:632:A:ALA:HB1  | 16       | 0.1           |
| (1,245) | 1:659:A:LYS:HB3  | 1:659:A:LYS:HA   | 17       | 0.1           |
| (1,230) | 1:604:A:VAL:HG21 | 1:604:A:VAL:HA   | 8        | 0.1           |
| (1,223) | 1:604:A:VAL:HG12 | 1:604:A:VAL:HA   | 4        | 0.1           |
| (1,223) | 1:604:A:VAL:HG13 | 1:604:A:VAL:HA   | 12       | 0.1           |
| (1,219) | 1:604:A:VAL:HA   | 1:607:A:LEU:HD22 | 11       | 0.1           |
| (1,191) | 1:601:A:SER:HB3  | 1:598:A:ASP:HA   | 13       | 0.1           |
| (1,140) | 1:643:A:ALA:HB3  | 1:640:A:TYR:HA   | 1        | 0.1           |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 4        | 0.1           |
| (1,68)  | 1:644:A:ASN:HD21 | 1:644:A:ASN:HA   | 13       | 0.1           |

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

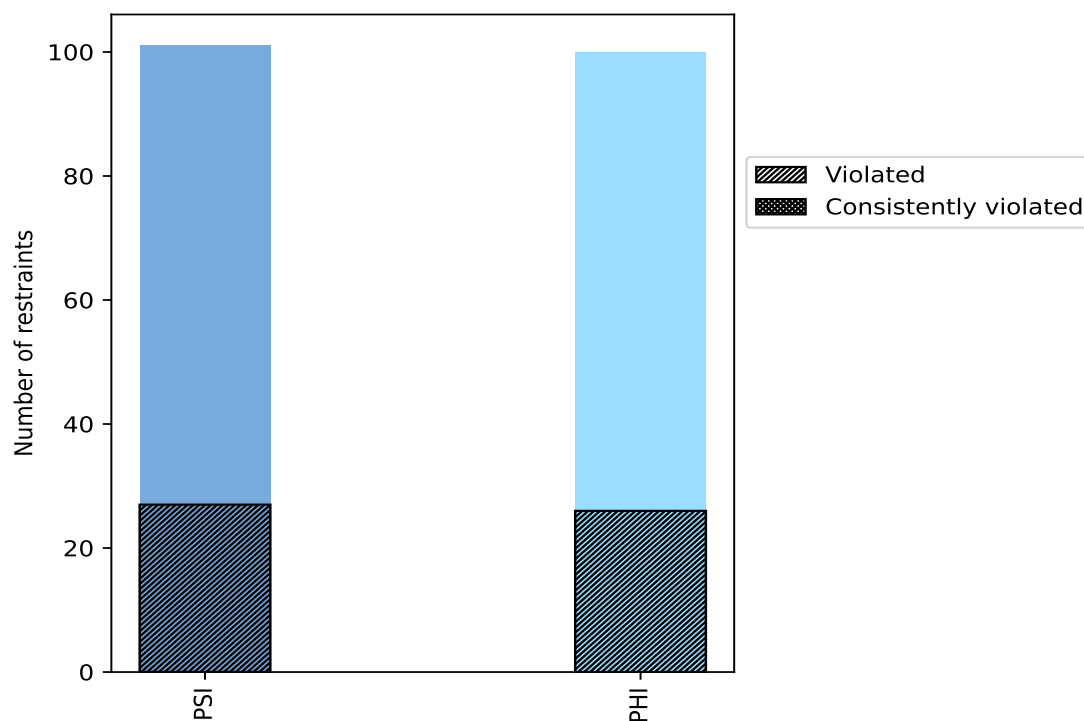
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 101   | 50.2           | 27                    | 26.7           | 13.4           | 0                                  | 0.0            | 0.0            |
| PHI        | 100   | 49.8           | 26                    | 26.0           | 12.9           | 0                                  | 0.0            | 0.0            |
| Total      | 201   | 100.0          | 53                    | 26.4           | 26.4           | 0                                  | 0.0            | 0.0            |

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

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



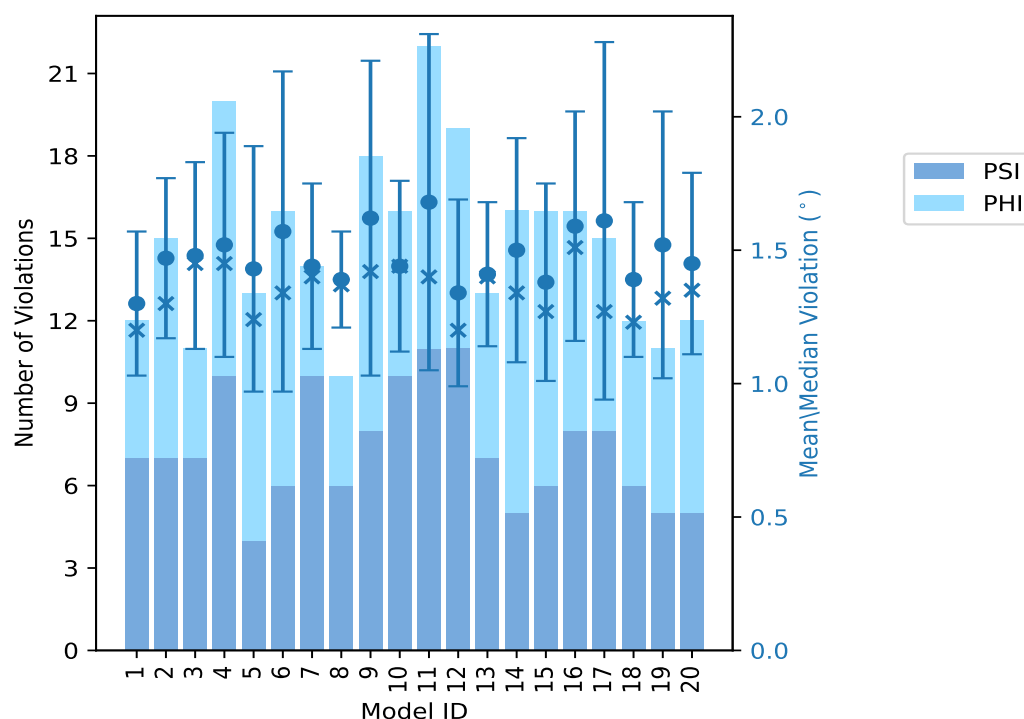
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 7                    | 5   | 12    | 1.3      | 1.94    | 0.27   | 1.2        |
| 2        | 7                    | 8   | 15    | 1.47     | 1.99    | 0.3    | 1.3        |
| 3        | 7                    | 4   | 11    | 1.48     | 1.93    | 0.35   | 1.45       |
| 4        | 10                   | 10  | 20    | 1.52     | 2.78    | 0.42   | 1.45       |
| 5        | 4                    | 9   | 13    | 1.43     | 2.69    | 0.46   | 1.24       |
| 6        | 6                    | 10  | 16    | 1.57     | 3.23    | 0.6    | 1.34       |
| 7        | 10                   | 4   | 14    | 1.44     | 2.12    | 0.31   | 1.4        |
| 8        | 6                    | 4   | 10    | 1.39     | 1.71    | 0.18   | 1.37       |
| 9        | 8                    | 10  | 18    | 1.62     | 3.56    | 0.59   | 1.42       |
| 10       | 10                   | 6   | 16    | 1.44     | 2.16    | 0.32   | 1.44       |
| 11       | 11                   | 11  | 22    | 1.68     | 3.68    | 0.63   | 1.4        |
| 12       | 11                   | 8   | 19    | 1.34     | 2.3     | 0.35   | 1.2        |
| 13       | 7                    | 6   | 13    | 1.41     | 1.92    | 0.27   | 1.4        |
| 14       | 5                    | 11  | 16    | 1.5      | 2.65    | 0.42   | 1.34       |
| 15       | 6                    | 10  | 16    | 1.38     | 2.59    | 0.37   | 1.27       |
| 16       | 8                    | 8   | 16    | 1.59     | 2.41    | 0.43   | 1.51       |
| 17       | 8                    | 7   | 15    | 1.61     | 3.39    | 0.67   | 1.27       |
| 18       | 6                    | 6   | 12    | 1.39     | 1.95    | 0.29   | 1.23       |
| 19       | 5                    | 6   | 11    | 1.52     | 2.74    | 0.5    | 1.32       |
| 20       | 5                    | 7   | 12    | 1.45     | 2.1     | 0.34   | 1.35       |

### 10.2.1 Bar graph : Dihedral 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

### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %    |
| 4                             | 8   | 12    | 1                        | 5.0  |
| 2                             | 1   | 3     | 2                        | 10.0 |
| 7                             | 1   | 8     | 3                        | 15.0 |
| 3                             | 3   | 6     | 4                        | 20.0 |
| 2                             | 2   | 4     | 5                        | 25.0 |
| 1                             | 0   | 1     | 6                        | 30.0 |
| 2                             | 2   | 4     | 7                        | 35.0 |
| 1                             | 2   | 3     | 8                        | 40.0 |
| 1                             | 1   | 2     | 9                        | 45.0 |
| 0                             | 2   | 2     | 10                       | 50.0 |
| 0                             | 0   | 0     | 11                       | 55.0 |

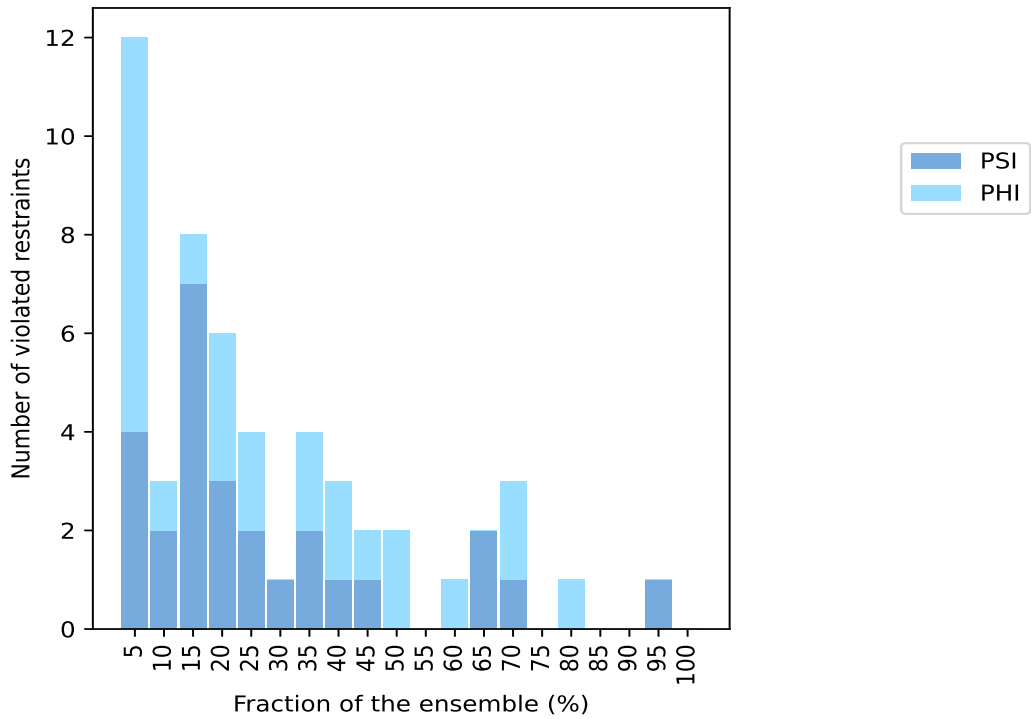
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 1   | 1     | 12                       | 60.0  |
| 2                             | 0   | 2     | 13                       | 65.0  |
| 1                             | 2   | 3     | 14                       | 70.0  |
| 0                             | 0   | 0     | 15                       | 75.0  |
| 0                             | 1   | 1     | 16                       | 80.0  |
| 0                             | 0   | 0     | 17                       | 85.0  |
| 0                             | 0   | 0     | 18                       | 90.0  |
| 1                             | 0   | 1     | 19                       | 95.0  |
| 0                             | 0   | 0     | 20                       | 100.0 |

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

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

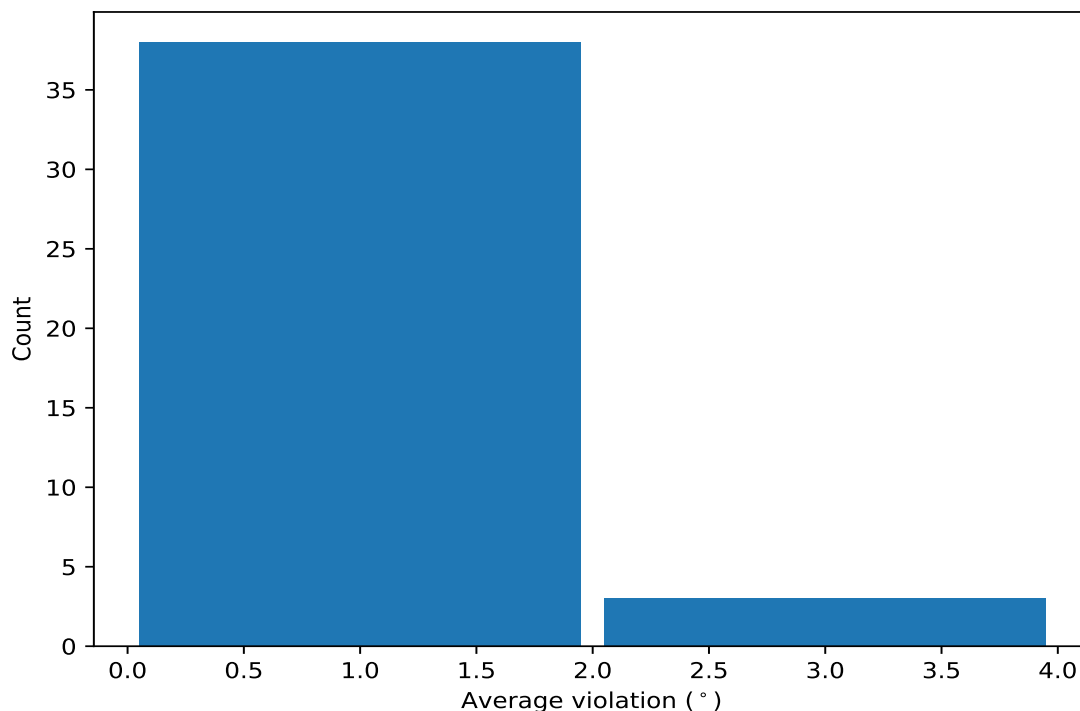


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



#### 10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 19                  | 1.71 | 0.38            | 1.71   |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 16                  | 1.55 | 0.24            | 1.52   |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 14                  | 1.42 | 0.25            | 1.34   |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 14                  | 1.29 | 0.21            | 1.27   |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 14                  | 1.28 | 0.21            | 1.19   |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 13                  | 1.91 | 0.39            | 1.9    |
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 13                  | 1.65 | 0.39            | 1.64   |
| (2,161) | 1:587:A:VAL:C | 1:588:A:ARG:N  | 1:588:A:ARG:CA | 1:588:A:ARG:C | 12                  | 1.71 | 0.26            | 1.76   |
| (1,8)   | 2:535:B:SER:C | 2:536:B:SER:N  | 2:536:B:SER:CA | 2:536:B:SER:C | 10                  | 1.46 | 0.38            | 1.3    |
| (1,30)  | 2:546:B:LEU:C | 2:547:B:SER:N  | 2:547:B:SER:CA | 2:547:B:SER:C | 10                  | 1.4  | 0.3             | 1.35   |
| (2,37)  | 1:606:A:LYS:C | 1:607:A:LEU:N  | 1:607:A:LEU:CA | 1:607:A:LEU:C | 9                   | 1.53 | 0.39            | 1.38   |
| (1,5)   | 2:534:B:PHE:N | 2:534:B:PHE:CA | 2:534:B:PHE:C  | 2:535:B:SER:N | 9                   | 1.47 | 0.48            | 1.22   |
| (2,12)  | 1:594:A:HIS:N | 1:594:A:HIS:CA | 1:594:A:HIS:C  | 1:595:A:VAL:N | 8                   | 1.47 | 0.31            | 1.42   |
| (2,25)  | 1:600:A:ARG:C | 1:601:A:SER:N  | 1:601:A:SER:CA | 1:601:A:SER:C | 8                   | 1.33 | 0.28            | 1.24   |
| (2,31)  | 1:603:A:LEU:C | 1:604:A:VAL:N  | 1:604:A:VAL:CA | 1:604:A:VAL:C | 8                   | 1.28 | 0.17            | 1.33   |
| (2,14)  | 1:595:A:VAL:N | 1:595:A:VAL:CA | 1:595:A:VAL:C  | 1:596:A:THR:N | 7                   | 2.57 | 0.75            | 2.59   |
| (2,15)  | 1:595:A:VAL:C | 1:596:A:THR:N  | 1:596:A:THR:CA | 1:596:A:THR:C | 7                   | 1.81 | 0.5             | 1.51   |
| (1,13)  | 2:538:B:ALA:N | 2:538:B:ALA:CA | 2:538:B:ALA:C  | 2:539:B:ASP:N | 7                   | 1.26 | 0.27            | 1.09   |
| (2,113) | 1:646:A:ARG:C | 1:647:A:ASP:N  | 1:647:A:ASP:CA | 1:647:A:ASP:C | 7                   | 1.14 | 0.09            | 1.14   |
| (1,31)  | 2:547:B:SER:N | 2:547:B:SER:CA | 2:547:B:SER:C  | 2:548:B:GLN:N | 6                   | 1.25 | 0.11            | 1.26   |

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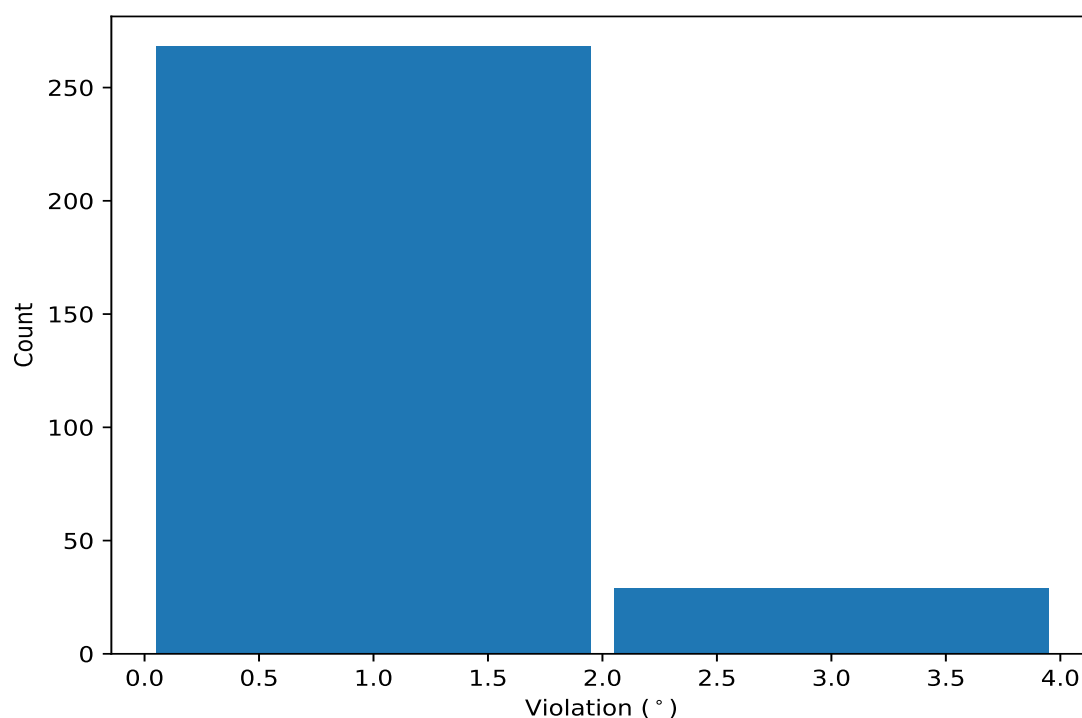
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (2,163) | 1:589:A:LYS:C | 1:590:A:GLY:N  | 1:590:A:GLY:CA | 1:590:A:GLY:C | 5                   | 2.18 | 0.85            | 2.65   |
| (2,16)  | 1:596:A:THR:N | 1:596:A:THR:CA | 1:596:A:THR:C  | 1:597:A:GLN:N | 5                   | 1.62 | 0.43            | 1.54   |
| (2,162) | 1:588:A:ARG:N | 1:588:A:ARG:CA | 1:588:A:ARG:C  | 1:589:A:LYS:N | 5                   | 1.37 | 0.29            | 1.6    |
| (2,85)  | 1:631:A:TYR:C | 1:632:A:ALA:N  | 1:632:A:ALA:CA | 1:632:A:ALA:C | 5                   | 1.26 | 0.14            | 1.3    |
| (2,4)   | 1:589:A:LYS:N | 1:589:A:LYS:CA | 1:589:A:LYS:C  | 1:590:A:GLY:N | 4                   | 2.3  | 0.74            | 1.98   |
| (2,89)  | 1:633:A:LYS:C | 1:634:A:LYS:N  | 1:634:A:LYS:CA | 1:634:A:LYS:C | 4                   | 1.6  | 0.38            | 1.67   |
| (2,142) | 1:661:A:GLN:N | 1:661:A:GLN:CA | 1:661:A:GLN:C  | 1:662:A:LYS:N | 4                   | 1.25 | 0.1             | 1.27   |
| (2,148) | 1:664:A:LEU:N | 1:664:A:LEU:CA | 1:664:A:LEU:C  | 1:665:A:GLU:N | 4                   | 1.22 | 0.1             | 1.25   |
| (2,135) | 1:657:A:ILE:C | 1:658:A:TYR:N  | 1:658:A:TYR:CA | 1:658:A:TYR:C | 4                   | 1.18 | 0.12            | 1.16   |
| (1,10)  | 2:536:B:SER:C | 2:537:B:ILE:N  | 2:537:B:ILE:CA | 2:537:B:ILE:C | 4                   | 1.17 | 0.07            | 1.19   |
| (2,164) | 1:590:A:GLY:N | 1:590:A:GLY:CA | 1:590:A:GLY:C  | 1:591:A:TRP:N | 3                   | 1.53 | 0.31            | 1.35   |
| (2,120) | 1:650:A:TYR:N | 1:650:A:TYR:CA | 1:650:A:TYR:C  | 1:651:A:HIS:N | 3                   | 1.37 | 0.04            | 1.37   |
| (2,94)  | 1:636:A:GLU:N | 1:636:A:GLU:CA | 1:636:A:GLU:C  | 1:637:A:GLY:N | 3                   | 1.22 | 0.1             | 1.28   |
| (1,25)  | 2:544:B:ALA:N | 2:544:B:ALA:CA | 2:544:B:ALA:C  | 2:545:B:LEU:N | 3                   | 1.18 | 0.14            | 1.12   |
| (2,154) | 1:667:A:LYS:N | 1:667:A:LYS:CA | 1:667:A:LYS:C  | 1:668:A:ARG:N | 3                   | 1.16 | 0.09            | 1.11   |
| (2,98)  | 1:638:A:ASP:N | 1:638:A:ASP:CA | 1:638:A:ASP:C  | 1:639:A:MET:N | 3                   | 1.14 | 0.02            | 1.14   |
| (1,22)  | 2:542:B:PHE:C | 2:543:B:SER:N  | 2:543:B:SER:CA | 2:543:B:SER:C | 3                   | 1.09 | 0.04            | 1.11   |
| (2,150) | 1:665:A:GLU:N | 1:665:A:GLU:CA | 1:665:A:GLU:C  | 1:666:A:GLU:N | 3                   | 1.08 | 0.03            | 1.07   |
| (2,62)  | 1:620:A:LEU:N | 1:620:A:LEU:CA | 1:620:A:LEU:C  | 1:621:A:LYS:N | 2                   | 1.66 | 0.06            | 1.66   |
| (2,64)  | 1:621:A:LYS:N | 1:621:A:LYS:CA | 1:621:A:LYS:C  | 1:622:A:ASP:N | 2                   | 1.23 | 0.02            | 1.23   |
| (1,4)   | 2:533:B:ASP:C | 2:534:B:PHE:N  | 2:534:B:PHE:CA | 2:534:B:PHE:C | 2                   | 1.18 | 0.1             | 1.18   |

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

## 10.5 All violated dihedral-angle restraints ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (2,14)  | 1:595:A:VAL:N | 1:595:A:VAL:CA | 1:595:A:VAL:C  | 1:596:A:THR:N | 11       | 3.68          |
| (2,4)   | 1:589:A:LYS:N | 1:589:A:LYS:CA | 1:589:A:LYS:C  | 1:590:A:GLY:N | 9        | 3.56          |
| (2,14)  | 1:595:A:VAL:N | 1:595:A:VAL:CA | 1:595:A:VAL:C  | 1:596:A:THR:N | 17       | 3.39          |
| (2,163) | 1:589:A:LYS:C | 1:590:A:GLY:N  | 1:590:A:GLY:CA | 1:590:A:GLY:C | 6        | 3.23          |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 4        | 2.78          |
| (1,5)   | 2:534:B:PHE:N | 2:534:B:PHE:CA | 2:534:B:PHE:C  | 2:535:B:SER:N | 19       | 2.74          |
| (2,163) | 1:589:A:LYS:C | 1:590:A:GLY:N  | 1:590:A:GLY:CA | 1:590:A:GLY:C | 5        | 2.69          |
| (2,14)  | 1:595:A:VAL:N | 1:595:A:VAL:CA | 1:595:A:VAL:C  | 1:596:A:THR:N | 6        | 2.66          |
| (2,163) | 1:589:A:LYS:C | 1:590:A:GLY:N  | 1:590:A:GLY:CA | 1:590:A:GLY:C | 14       | 2.65          |
| (2,15)  | 1:595:A:VAL:C | 1:596:A:THR:N  | 1:596:A:THR:CA | 1:596:A:THR:C | 11       | 2.61          |
| (2,14)  | 1:595:A:VAL:N | 1:595:A:VAL:CA | 1:595:A:VAL:C  | 1:596:A:THR:N | 15       | 2.59          |
| (2,15)  | 1:595:A:VAL:C | 1:596:A:THR:N  | 1:596:A:THR:CA | 1:596:A:THR:C | 17       | 2.53          |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 17       | 2.49          |
| (2,14)  | 1:595:A:VAL:N | 1:595:A:VAL:CA | 1:595:A:VAL:C  | 1:596:A:THR:N | 9        | 2.46          |
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 16       | 2.41          |
| (2,37)  | 1:606:A:LYS:C | 1:607:A:LEU:N  | 1:607:A:LEU:CA | 1:607:A:LEU:C | 11       | 2.3           |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 12       | 2.3           |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 11       | 2.26          |
| (1,8)   | 2:535:B:SER:C | 2:536:B:SER:N  | 2:536:B:SER:CA | 2:536:B:SER:C | 16       | 2.26          |
| (2,16)  | 1:596:A:THR:N | 1:596:A:THR:CA | 1:596:A:THR:C  | 1:597:A:GLN:N | 11       | 2.24          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 16       | 2.16          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 10       | 2.16          |
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 19       | 2.14          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 7        | 2.12          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 20       | 2.1           |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 9        | 2.09          |
| (2,161) | 1:587:A:VAL:C | 1:588:A:ARG:N  | 1:588:A:ARG:CA | 1:588:A:ARG:C | 12       | 2.08          |
| (2,4)   | 1:589:A:LYS:N | 1:589:A:LYS:CA | 1:589:A:LYS:C  | 1:590:A:GLY:N | 6        | 2.05          |
| (2,89)  | 1:633:A:LYS:C | 1:634:A:LYS:N  | 1:634:A:LYS:CA | 1:634:A:LYS:C | 14       | 2.02          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 2        | 1.99          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 10       | 1.99          |
| (2,16)  | 1:596:A:THR:N | 1:596:A:THR:CA | 1:596:A:THR:C  | 1:597:A:GLN:N | 20       | 1.99          |
| (2,164) | 1:590:A:GLY:N | 1:590:A:GLY:CA | 1:590:A:GLY:C  | 1:591:A:TRP:N | 11       | 1.96          |
| (1,30)  | 2:546:B:LEU:C | 2:547:B:SER:N  | 2:547:B:SER:CA | 2:547:B:SER:C | 4        | 1.96          |
| (1,8)   | 2:535:B:SER:C | 2:536:B:SER:N  | 2:536:B:SER:CA | 2:536:B:SER:C | 7        | 1.96          |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 11       | 1.96          |
| (2,161) | 1:587:A:VAL:C | 1:588:A:ARG:N  | 1:588:A:ARG:CA | 1:588:A:ARG:C | 2        | 1.95          |
| (2,161) | 1:587:A:VAL:C | 1:588:A:ARG:N  | 1:588:A:ARG:CA | 1:588:A:ARG:C | 11       | 1.95          |
| (2,12)  | 1:594:A:HIS:N | 1:594:A:HIS:CA | 1:594:A:HIS:C  | 1:595:A:VAL:N | 18       | 1.95          |
| (2,161) | 1:587:A:VAL:C | 1:588:A:ARG:N  | 1:588:A:ARG:CA | 1:588:A:ARG:C | 16       | 1.94          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 20       | 1.94          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 1        | 1.94          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 3        | 1.93          |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 18       | 1.92          |
| (2,4)   | 1:589:A:LYS:N | 1:589:A:LYS:CA | 1:589:A:LYS:C  | 1:590:A:GLY:N | 5        | 1.92          |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 3        | 1.92          |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 13       | 1.92          |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 9        | 1.9           |
| (2,161) | 1:587:A:VAL:C | 1:588:A:ARG:N  | 1:588:A:ARG:CA | 1:588:A:ARG:C | 9        | 1.87          |
| (2,89)  | 1:633:A:LYS:C | 1:634:A:LYS:N  | 1:634:A:LYS:CA | 1:634:A:LYS:C | 4        | 1.87          |
| (2,14)  | 1:595:A:VAL:N | 1:595:A:VAL:CA | 1:595:A:VAL:C  | 1:596:A:THR:N | 3        | 1.87          |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 16       | 1.87          |
| (2,161) | 1:587:A:VAL:C | 1:588:A:ARG:N  | 1:588:A:ARG:CA | 1:588:A:ARG:C | 17       | 1.86          |
| (2,25)  | 1:600:A:ARG:C | 1:601:A:SER:N  | 1:601:A:SER:CA | 1:601:A:SER:C | 14       | 1.84          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 19       | 1.82          |
| (2,37)  | 1:606:A:LYS:C | 1:607:A:LEU:N  | 1:607:A:LEU:CA | 1:607:A:LEU:C | 16       | 1.81          |
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 4        | 1.81          |
| (2,12)  | 1:594:A:HIS:N | 1:594:A:HIS:CA | 1:594:A:HIS:C  | 1:595:A:VAL:N | 14       | 1.81          |
| (1,30)  | 2:546:B:LEU:C | 2:547:B:SER:N  | 2:547:B:SER:CA | 2:547:B:SER:C | 2        | 1.81          |
| (2,37)  | 1:606:A:LYS:C | 1:607:A:LEU:N  | 1:607:A:LEU:CA | 1:607:A:LEU:C | 15       | 1.8           |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 6        | 1.79          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 4        | 1.78          |
| (2,37)  | 1:606:A:LYS:C | 1:607:A:LEU:N  | 1:607:A:LEU:CA | 1:607:A:LEU:C | 2        | 1.78          |
| (2,15)  | 1:595:A:VAL:C | 1:596:A:THR:N  | 1:596:A:THR:CA | 1:596:A:THR:C | 15       | 1.78          |
| (1,13)  | 2:538:B:ALA:N | 2:538:B:ALA:CA | 2:538:B:ALA:C  | 2:539:B:ASP:N | 4        | 1.76          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 13       | 1.74          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 6        | 1.74          |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 4        | 1.74          |
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 2        | 1.74          |
| (1,8)   | 2:535:B:SER:C | 2:536:B:SER:N  | 2:536:B:SER:CA | 2:536:B:SER:C | 4        | 1.74          |
| (2,62)  | 1:620:A:LEU:N | 1:620:A:LEU:CA | 1:620:A:LEU:C  | 1:621:A:LYS:N | 3        | 1.73          |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 8        | 1.71          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 13       | 1.71          |
| (2,12)  | 1:594:A:HIS:N | 1:594:A:HIS:CA | 1:594:A:HIS:C  | 1:595:A:VAL:N | 5        | 1.7           |
| (2,25)  | 1:600:A:ARG:C | 1:601:A:SER:N  | 1:601:A:SER:CA | 1:601:A:SER:C | 10       | 1.69          |
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 11       | 1.69          |
| (2,4)   | 1:589:A:LYS:N | 1:589:A:LYS:CA | 1:589:A:LYS:C  | 1:590:A:GLY:N | 14       | 1.69          |
| (1,5)   | 2:534:B:PHE:N | 2:534:B:PHE:CA | 2:534:B:PHE:C  | 2:535:B:SER:N | 14       | 1.69          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 18       | 1.68          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 3        | 1.68          |
| (2,161) | 1:587:A:VAL:C | 1:588:A:ARG:N  | 1:588:A:ARG:CA | 1:588:A:ARG:C | 5        | 1.67          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 12       | 1.67          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 8        | 1.66          |
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 17       | 1.64          |
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 6        | 1.63          |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 10       | 1.62          |
| (2,162) | 1:588:A:ARG:N | 1:588:A:ARG:CA | 1:588:A:ARG:C  | 1:589:A:LYS:N | 4        | 1.61          |
| (2,162) | 1:588:A:ARG:N | 1:588:A:ARG:CA | 1:588:A:ARG:C  | 1:589:A:LYS:N | 7        | 1.61          |
| (2,162) | 1:588:A:ARG:N | 1:588:A:ARG:CA | 1:588:A:ARG:C  | 1:589:A:LYS:N | 12       | 1.6           |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 16       | 1.6           |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 7        | 1.6           |
| (2,62)  | 1:620:A:LEU:N | 1:620:A:LEU:CA | 1:620:A:LEU:C  | 1:621:A:LYS:N | 7        | 1.6           |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 1        | 1.6           |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 10       | 1.59          |
| (1,30)  | 2:546:B:LEU:C | 2:547:B:SER:N  | 2:547:B:SER:CA | 2:547:B:SER:C | 10       | 1.59          |
| (2,161) | 1:587:A:VAL:C | 1:588:A:ARG:N  | 1:588:A:ARG:CA | 1:588:A:ARG:C | 13       | 1.57          |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 14       | 1.57          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 17       | 1.57          |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 2        | 1.57          |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 1        | 1.56          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 19       | 1.56          |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 5        | 1.55          |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 16       | 1.55          |
| (2,12)  | 1:594:A:HIS:N | 1:594:A:HIS:CA | 1:594:A:HIS:C  | 1:595:A:VAL:N | 12       | 1.55          |
| (2,16)  | 1:596:A:THR:N | 1:596:A:THR:CA | 1:596:A:THR:C  | 1:597:A:GLN:N | 17       | 1.54          |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 18       | 1.54          |
| (2,161) | 1:587:A:VAL:C | 1:588:A:ARG:N  | 1:588:A:ARG:CA | 1:588:A:ARG:C | 7        | 1.53          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 9        | 1.53          |
| (1,13)  | 2:538:B:ALA:N | 2:538:B:ALA:CA | 2:538:B:ALA:C  | 2:539:B:ASP:N | 13       | 1.53          |
| (2,161) | 1:587:A:VAL:C | 1:588:A:ARG:N  | 1:588:A:ARG:CA | 1:588:A:ARG:C | 4        | 1.52          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 10       | 1.52          |
| (1,5)   | 2:534:B:PHE:N | 2:534:B:PHE:CA | 2:534:B:PHE:C  | 2:535:B:SER:N | 9        | 1.52          |
| (2,15)  | 1:595:A:VAL:C | 1:596:A:THR:N  | 1:596:A:THR:CA | 1:596:A:THR:C | 6        | 1.51          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 8        | 1.5           |
| (1,30)  | 2:546:B:LEU:C | 2:547:B:SER:N  | 2:547:B:SER:CA | 2:547:B:SER:C | 11       | 1.5           |
| (2,31)  | 1:603:A:LEU:C | 1:604:A:VAL:N  | 1:604:A:VAL:CA | 1:604:A:VAL:C | 2        | 1.49          |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 1        | 1.48          |
| (2,31)  | 1:603:A:LEU:C | 1:604:A:VAL:N  | 1:604:A:VAL:CA | 1:604:A:VAL:C | 20       | 1.48          |
| (2,89)  | 1:633:A:LYS:C | 1:634:A:LYS:N  | 1:634:A:LYS:CA | 1:634:A:LYS:C | 16       | 1.47          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 10       | 1.47          |
| (2,15)  | 1:595:A:VAL:C | 1:596:A:THR:N  | 1:596:A:THR:CA | 1:596:A:THR:C | 3        | 1.45          |
| (2,15)  | 1:595:A:VAL:C | 1:596:A:THR:N  | 1:596:A:THR:CA | 1:596:A:THR:C | 9        | 1.45          |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 9        | 1.44          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (2,120) | 1:650:A:TYR:N | 1:650:A:TYR:CA | 1:650:A:TYR:C  | 1:651:A:HIS:N | 16       | 1.43          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 7        | 1.43          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 11       | 1.43          |
| (2,25)  | 1:600:A:ARG:C | 1:601:A:SER:N  | 1:601:A:SER:CA | 1:601:A:SER:C | 19       | 1.43          |
| (1,31)  | 2:547:B:SER:N | 2:547:B:SER:CA | 2:547:B:SER:C  | 2:548:B:GLN:N | 8        | 1.43          |
| (1,8)   | 2:535:B:SER:C | 2:536:B:SER:N  | 2:536:B:SER:CA | 2:536:B:SER:C | 13       | 1.43          |
| (2,85)  | 1:631:A:TYR:C | 1:632:A:ALA:N  | 1:632:A:ALA:CA | 1:632:A:ALA:C | 14       | 1.41          |
| (1,1)   | 2:532:B:GLU:N | 2:532:B:GLU:CA | 2:532:B:GLU:C  | 2:533:B:ASP:N | 8        | 1.41          |
| (2,161) | 1:587:A:VAL:C | 1:588:A:ARG:N  | 1:588:A:ARG:CA | 1:588:A:ARG:C | 6        | 1.4           |
| (2,138) | 1:659:A:LYS:N | 1:659:A:LYS:CA | 1:659:A:LYS:C  | 1:660:A:ILE:N | 10       | 1.4           |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 13       | 1.4           |
| (2,31)  | 1:603:A:LEU:C | 1:604:A:VAL:N  | 1:604:A:VAL:CA | 1:604:A:VAL:C | 9        | 1.4           |
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 12       | 1.4           |
| (2,85)  | 1:631:A:TYR:C | 1:632:A:ALA:N  | 1:632:A:ALA:CA | 1:632:A:ALA:C | 4        | 1.38          |
| (2,37)  | 1:606:A:LYS:C | 1:607:A:LEU:N  | 1:607:A:LEU:CA | 1:607:A:LEU:C | 20       | 1.38          |
| (2,120) | 1:650:A:TYR:N | 1:650:A:TYR:CA | 1:650:A:TYR:C  | 1:651:A:HIS:N | 15       | 1.37          |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 7        | 1.37          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 4        | 1.37          |
| (1,30)  | 2:546:B:LEU:C | 2:547:B:SER:N  | 2:547:B:SER:CA | 2:547:B:SER:C | 18       | 1.37          |
| (1,25)  | 2:544:B:ALA:N | 2:544:B:ALA:CA | 2:544:B:ALA:C  | 2:545:B:LEU:N | 13       | 1.37          |
| (2,142) | 1:661:A:GLN:N | 1:661:A:GLN:CA | 1:661:A:GLN:C  | 1:662:A:LYS:N | 7        | 1.36          |
| (2,135) | 1:657:A:ILE:C | 1:658:A:TYR:N  | 1:658:A:TYR:CA | 1:658:A:TYR:C | 9        | 1.36          |
| (1,13)  | 2:538:B:ALA:N | 2:538:B:ALA:CA | 2:538:B:ALA:C  | 2:539:B:ASP:N | 11       | 1.36          |
| (2,164) | 1:590:A:GLY:N | 1:590:A:GLY:CA | 1:590:A:GLY:C  | 1:591:A:TRP:N | 20       | 1.35          |
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 1        | 1.34          |
| (2,14)  | 1:595:A:VAL:N | 1:595:A:VAL:CA | 1:595:A:VAL:C  | 1:596:A:THR:N | 20       | 1.34          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 11       | 1.33          |
| (2,31)  | 1:603:A:LEU:C | 1:604:A:VAL:N  | 1:604:A:VAL:CA | 1:604:A:VAL:C | 8        | 1.33          |
| (2,31)  | 1:603:A:LEU:C | 1:604:A:VAL:N  | 1:604:A:VAL:CA | 1:604:A:VAL:C | 12       | 1.33          |
| (1,30)  | 2:546:B:LEU:C | 2:547:B:SER:N  | 2:547:B:SER:CA | 2:547:B:SER:C | 15       | 1.33          |
| (1,8)   | 2:535:B:SER:C | 2:536:B:SER:N  | 2:536:B:SER:CA | 2:536:B:SER:C | 11       | 1.33          |
| (2,148) | 1:664:A:LEU:N | 1:664:A:LEU:CA | 1:664:A:LEU:C  | 1:665:A:GLU:N | 12       | 1.32          |
| (2,120) | 1:650:A:TYR:N | 1:650:A:TYR:CA | 1:650:A:TYR:C  | 1:651:A:HIS:N | 19       | 1.32          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 5        | 1.32          |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 4        | 1.32          |
| (2,37)  | 1:606:A:LYS:C | 1:607:A:LEU:N  | 1:607:A:LEU:CA | 1:607:A:LEU:C | 8        | 1.32          |
| (2,94)  | 1:636:A:GLU:N | 1:636:A:GLU:CA | 1:636:A:GLU:C  | 1:637:A:GLY:N | 16       | 1.31          |
| (2,15)  | 1:595:A:VAL:C | 1:596:A:THR:N  | 1:596:A:THR:CA | 1:596:A:THR:C | 20       | 1.31          |
| (2,142) | 1:661:A:GLN:N | 1:661:A:GLN:CA | 1:661:A:GLN:C  | 1:662:A:LYS:N | 13       | 1.3           |
| (2,85)  | 1:631:A:TYR:C | 1:632:A:ALA:N  | 1:632:A:ALA:CA | 1:632:A:ALA:C | 2        | 1.3           |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 15       | 1.3           |
| (2,148) | 1:664:A:LEU:N | 1:664:A:LEU:CA | 1:664:A:LEU:C  | 1:665:A:GLU:N | 2        | 1.29          |
| (2,112) | 1:646:A:ARG:N | 1:646:A:ARG:CA | 1:646:A:ARG:C  | 1:647:A:ASP:N | 12       | 1.29          |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 9        | 1.29          |
| (1,5)   | 2:534:B:PHE:N | 2:534:B:PHE:CA | 2:534:B:PHE:C  | 2:535:B:SER:N | 3        | 1.29          |
| (2,154) | 1:667:A:LYS:N | 1:667:A:LYS:CA | 1:667:A:LYS:C  | 1:668:A:ARG:N | 11       | 1.28          |
| (2,113) | 1:646:A:ARG:C | 1:647:A:ASP:N  | 1:647:A:ASP:CA | 1:647:A:ASP:C | 6        | 1.28          |
| (2,94)  | 1:636:A:GLU:N | 1:636:A:GLU:CA | 1:636:A:GLU:C  | 1:637:A:GLY:N | 14       | 1.28          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 15       | 1.28          |
| (2,53)  | 1:615:A:PRO:C | 1:616:A:ASP:N  | 1:616:A:ASP:CA | 1:616:A:ASP:C | 15       | 1.28          |
| (2,37)  | 1:606:A:LYS:C | 1:607:A:LEU:N  | 1:607:A:LEU:CA | 1:607:A:LEU:C | 9        | 1.28          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (2,12)  | 1:594:A:HIS:N | 1:594:A:HIS:CA | 1:594:A:HIS:C  | 1:595:A:VAL:N | 4        | 1.28          |
| (1,31)  | 2:547:B:SER:N | 2:547:B:SER:CA | 2:547:B:SER:C  | 2:548:B:GLN:N | 16       | 1.28          |
| (1,4)   | 2:533:B:ASP:C | 2:534:B:PHE:N  | 2:534:B:PHE:CA | 2:534:B:PHE:C | 6        | 1.28          |
| (2,164) | 1:590:A:GLY:N | 1:590:A:GLY:CA | 1:590:A:GLY:C  | 1:591:A:TRP:N | 17       | 1.27          |
| (1,31)  | 2:547:B:SER:N | 2:547:B:SER:CA | 2:547:B:SER:C  | 2:548:B:GLN:N | 9        | 1.27          |
| (1,30)  | 2:546:B:LEU:C | 2:547:B:SER:N  | 2:547:B:SER:CA | 2:547:B:SER:C | 1        | 1.27          |
| (1,8)   | 2:535:B:SER:C | 2:536:B:SER:N  | 2:536:B:SER:CA | 2:536:B:SER:C | 15       | 1.27          |
| (2,25)  | 1:600:A:ARG:C | 1:601:A:SER:N  | 1:601:A:SER:CA | 1:601:A:SER:C | 11       | 1.26          |
| (1,12)  | 2:537:B:ILE:C | 2:538:B:ALA:N  | 2:538:B:ALA:CA | 2:538:B:ALA:C | 9        | 1.26          |
| (1,8)   | 2:535:B:SER:C | 2:536:B:SER:N  | 2:536:B:SER:CA | 2:536:B:SER:C | 19       | 1.26          |
| (2,64)  | 1:621:A:LYS:N | 1:621:A:LYS:CA | 1:621:A:LYS:C  | 1:622:A:ASP:N | 3        | 1.25          |
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 9        | 1.25          |
| (1,31)  | 2:547:B:SER:N | 2:547:B:SER:CA | 2:547:B:SER:C  | 2:548:B:GLN:N | 10       | 1.25          |
| (2,163) | 1:589:A:LYS:C | 1:590:A:GLY:N  | 1:590:A:GLY:CA | 1:590:A:GLY:C | 2        | 1.24          |
| (2,142) | 1:661:A:GLN:N | 1:661:A:GLN:CA | 1:661:A:GLN:C  | 1:662:A:LYS:N | 11       | 1.24          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 6        | 1.24          |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 5        | 1.24          |
| (2,12)  | 1:594:A:HIS:N | 1:594:A:HIS:CA | 1:594:A:HIS:C  | 1:595:A:VAL:N | 19       | 1.24          |
| (1,10)  | 2:536:B:SER:C | 2:537:B:ILE:N  | 2:537:B:ILE:CA | 2:537:B:ILE:C | 6        | 1.24          |
| (2,113) | 1:646:A:ARG:C | 1:647:A:ASP:N  | 1:647:A:ASP:CA | 1:647:A:ASP:C | 20       | 1.23          |
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 17       | 1.23          |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 15       | 1.23          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 18       | 1.23          |
| (1,31)  | 2:547:B:SER:N | 2:547:B:SER:CA | 2:547:B:SER:C  | 2:548:B:GLN:N | 15       | 1.23          |
| (2,148) | 1:664:A:LEU:N | 1:664:A:LEU:CA | 1:664:A:LEU:C  | 1:665:A:GLU:N | 10       | 1.22          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 2        | 1.22          |
| (2,25)  | 1:600:A:ARG:C | 1:601:A:SER:N  | 1:601:A:SER:CA | 1:601:A:SER:C | 18       | 1.22          |
| (1,5)   | 2:534:B:PHE:N | 2:534:B:PHE:CA | 2:534:B:PHE:C  | 2:535:B:SER:N | 10       | 1.22          |
| (2,157) | 1:668:A:ARG:C | 1:669:A:ARG:N  | 1:669:A:ARG:CA | 1:669:A:ARG:C | 11       | 1.21          |
| (2,143) | 1:661:A:GLN:C | 1:662:A:LYS:N  | 1:662:A:LYS:CA | 1:662:A:LYS:C | 14       | 1.21          |
| (2,64)  | 1:621:A:LYS:N | 1:621:A:LYS:CA | 1:621:A:LYS:C  | 1:622:A:ASP:N | 7        | 1.21          |
| (1,5)   | 2:534:B:PHE:N | 2:534:B:PHE:CA | 2:534:B:PHE:C  | 2:535:B:SER:N | 15       | 1.21          |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 12       | 1.2           |
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 8        | 1.2           |
| (1,5)   | 2:534:B:PHE:N | 2:534:B:PHE:CA | 2:534:B:PHE:C  | 2:535:B:SER:N | 7        | 1.2           |
| (1,5)   | 2:534:B:PHE:N | 2:534:B:PHE:CA | 2:534:B:PHE:C  | 2:535:B:SER:N | 18       | 1.2           |
| (2,135) | 1:657:A:ILE:C | 1:658:A:TYR:N  | 1:658:A:TYR:CA | 1:658:A:TYR:C | 18       | 1.19          |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 2        | 1.19          |
| (1,10)  | 2:536:B:SER:C | 2:537:B:ILE:N  | 2:537:B:ILE:CA | 2:537:B:ILE:C | 14       | 1.19          |
| (1,10)  | 2:536:B:SER:C | 2:537:B:ILE:N  | 2:537:B:ILE:CA | 2:537:B:ILE:C | 18       | 1.19          |
| (1,8)   | 2:535:B:SER:C | 2:536:B:SER:N  | 2:536:B:SER:CA | 2:536:B:SER:C | 14       | 1.19          |
| (1,5)   | 2:534:B:PHE:N | 2:534:B:PHE:CA | 2:534:B:PHE:C  | 2:535:B:SER:N | 2        | 1.19          |
| (2,161) | 1:587:A:VAL:C | 1:588:A:ARG:N  | 1:588:A:ARG:CA | 1:588:A:ARG:C | 15       | 1.17          |
| (2,113) | 1:646:A:ARG:C | 1:647:A:ASP:N  | 1:647:A:ASP:CA | 1:647:A:ASP:C | 11       | 1.17          |
| (2,98)  | 1:638:A:ASP:N | 1:638:A:ASP:CA | 1:638:A:ASP:C  | 1:639:A:MET:N | 2        | 1.17          |
| (2,85)  | 1:631:A:TYR:C | 1:632:A:ALA:N  | 1:632:A:ALA:CA | 1:632:A:ALA:C | 5        | 1.17          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 8        | 1.17          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 14       | 1.17          |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 11       | 1.17          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 18       | 1.17          |
| (2,16)  | 1:596:A:THR:N | 1:596:A:THR:CA | 1:596:A:THR:C  | 1:597:A:GLN:N | 13       | 1.17          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (2,109) | 1:644:A:ASN:C | 1:645:A:SER:N  | 1:645:A:SER:CA | 1:645:A:SER:C | 15       | 1.16          |
| (2,16)  | 1:596:A:THR:N | 1:596:A:THR:CA | 1:596:A:THR:C  | 1:597:A:GLN:N | 8        | 1.16          |
| (2,35)  | 1:605:A:HIS:C | 1:606:A:LYS:N  | 1:606:A:LYS:CA | 1:606:A:LYS:C | 14       | 1.15          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 5        | 1.15          |
| (2,135) | 1:657:A:ILE:C | 1:658:A:TYR:N  | 1:658:A:TYR:CA | 1:658:A:TYR:C | 20       | 1.14          |
| (2,113) | 1:646:A:ARG:C | 1:647:A:ASP:N  | 1:647:A:ASP:CA | 1:647:A:ASP:C | 15       | 1.14          |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 20       | 1.14          |
| (2,98)  | 1:638:A:ASP:N | 1:638:A:ASP:CA | 1:638:A:ASP:C  | 1:639:A:MET:N | 12       | 1.14          |
| (2,92)  | 1:635:A:VAL:N | 1:635:A:VAL:CA | 1:635:A:VAL:C  | 1:636:A:GLU:N | 13       | 1.14          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 4        | 1.14          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 9        | 1.14          |
| (2,25)  | 1:600:A:ARG:C | 1:601:A:SER:N  | 1:601:A:SER:CA | 1:601:A:SER:C | 17       | 1.14          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 17       | 1.13          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 12       | 1.13          |
| (2,12)  | 1:594:A:HIS:N | 1:594:A:HIS:CA | 1:594:A:HIS:C  | 1:595:A:VAL:N | 1        | 1.13          |
| (1,22)  | 2:542:B:PHE:C | 2:543:B:SER:N  | 2:543:B:SER:CA | 2:543:B:SER:C | 19       | 1.13          |
| (2,150) | 1:665:A:GLU:N | 1:665:A:GLU:CA | 1:665:A:GLU:C  | 1:666:A:GLU:N | 10       | 1.12          |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 17       | 1.12          |
| (2,98)  | 1:638:A:ASP:N | 1:638:A:ASP:CA | 1:638:A:ASP:C  | 1:639:A:MET:N | 17       | 1.12          |
| (2,31)  | 1:603:A:LEU:C | 1:604:A:VAL:N  | 1:604:A:VAL:CA | 1:604:A:VAL:C | 10       | 1.12          |
| (1,25)  | 2:544:B:ALA:N | 2:544:B:ALA:CA | 2:544:B:ALA:C  | 2:545:B:LEU:N | 12       | 1.12          |
| (2,163) | 1:589:A:LYS:C | 1:590:A:GLY:N  | 1:590:A:GLY:CA | 1:590:A:GLY:C | 16       | 1.11          |
| (2,154) | 1:667:A:LYS:N | 1:667:A:LYS:CA | 1:667:A:LYS:C  | 1:668:A:ARG:N | 4        | 1.11          |
| (2,17)  | 1:596:A:THR:C | 1:597:A:GLN:N  | 1:597:A:GLN:CA | 1:597:A:GLN:C | 12       | 1.11          |
| (1,22)  | 2:542:B:PHE:C | 2:543:B:SER:N  | 2:543:B:SER:CA | 2:543:B:SER:C | 5        | 1.11          |
| (2,142) | 1:661:A:GLN:N | 1:661:A:GLN:CA | 1:661:A:GLN:C  | 1:662:A:LYS:N | 1        | 1.1           |
| (1,30)  | 2:546:B:LEU:C | 2:547:B:SER:N  | 2:547:B:SER:CA | 2:547:B:SER:C | 16       | 1.1           |
| (2,154) | 1:667:A:LYS:N | 1:667:A:LYS:CA | 1:667:A:LYS:C  | 1:668:A:ARG:N | 1        | 1.09          |
| (2,31)  | 1:603:A:LEU:C | 1:604:A:VAL:N  | 1:604:A:VAL:CA | 1:604:A:VAL:C | 11       | 1.09          |
| (2,12)  | 1:594:A:HIS:N | 1:594:A:HIS:CA | 1:594:A:HIS:C  | 1:595:A:VAL:N | 7        | 1.09          |
| (1,13)  | 2:538:B:ALA:N | 2:538:B:ALA:CA | 2:538:B:ALA:C  | 2:539:B:ASP:N | 16       | 1.09          |
| (1,8)   | 2:535:B:SER:C | 2:536:B:SER:N  | 2:536:B:SER:CA | 2:536:B:SER:C | 12       | 1.09          |
| (2,140) | 1:660:A:ILE:N | 1:660:A:ILE:CA | 1:660:A:ILE:C  | 1:661:A:GLN:N | 10       | 1.08          |
| (2,113) | 1:646:A:ARG:C | 1:647:A:ASP:N  | 1:647:A:ASP:CA | 1:647:A:ASP:C | 1        | 1.08          |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 14       | 1.08          |
| (2,94)  | 1:636:A:GLU:N | 1:636:A:GLU:CA | 1:636:A:GLU:C  | 1:637:A:GLY:N | 4        | 1.08          |
| (2,37)  | 1:606:A:LYS:C | 1:607:A:LEU:N  | 1:607:A:LEU:CA | 1:607:A:LEU:C | 4        | 1.08          |
| (2,150) | 1:665:A:GLU:N | 1:665:A:GLU:CA | 1:665:A:GLU:C  | 1:666:A:GLU:N | 18       | 1.07          |
| (2,113) | 1:646:A:ARG:C | 1:647:A:ASP:N  | 1:647:A:ASP:CA | 1:647:A:ASP:C | 13       | 1.07          |
| (1,13)  | 2:538:B:ALA:N | 2:538:B:ALA:CA | 2:538:B:ALA:C  | 2:539:B:ASP:N | 7        | 1.07          |
| (1,4)   | 2:533:B:ASP:C | 2:534:B:PHE:N  | 2:534:B:PHE:CA | 2:534:B:PHE:C | 2        | 1.07          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 19       | 1.06          |
| (2,74)  | 1:626:A:GLU:N | 1:626:A:GLU:CA | 1:626:A:GLU:C  | 1:627:A:ASN:N | 6        | 1.06          |
| (2,37)  | 1:606:A:LYS:C | 1:607:A:LEU:N  | 1:607:A:LEU:CA | 1:607:A:LEU:C | 6        | 1.06          |
| (2,18)  | 1:597:A:GLN:N | 1:597:A:GLN:CA | 1:597:A:GLN:C  | 1:598:A:ASP:N | 7        | 1.06          |
| (1,10)  | 2:536:B:SER:C | 2:537:B:ILE:N  | 2:537:B:ILE:CA | 2:537:B:ILE:C | 17       | 1.06          |
| (1,2)   | 2:532:B:GLU:C | 2:533:B:ASP:N  | 2:533:B:ASP:CA | 2:533:B:ASP:C | 5        | 1.06          |
| (2,148) | 1:664:A:LEU:N | 1:664:A:LEU:CA | 1:664:A:LEU:C  | 1:665:A:GLU:N | 4        | 1.05          |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 12       | 1.05          |
| (2,25)  | 1:600:A:ARG:C | 1:601:A:SER:N  | 1:601:A:SER:CA | 1:601:A:SER:C | 1        | 1.05          |
| (1,30)  | 2:546:B:LEU:C | 2:547:B:SER:N  | 2:547:B:SER:CA | 2:547:B:SER:C | 3        | 1.05          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,8)   | 2:535:B:SER:C | 2:536:B:SER:N  | 2:536:B:SER:CA | 2:536:B:SER:C | 3        | 1.05          |
| (2,150) | 1:665:A:GLU:N | 1:665:A:GLU:CA | 1:665:A:GLU:C  | 1:666:A:GLU:N | 16       | 1.04          |
| (2,135) | 1:657:A:ILE:C | 1:658:A:TYR:N  | 1:658:A:TYR:CA | 1:658:A:TYR:C | 5        | 1.04          |
| (2,89)  | 1:633:A:LYS:C | 1:634:A:LYS:N  | 1:634:A:LYS:CA | 1:634:A:LYS:C | 9        | 1.04          |
| (2,25)  | 1:600:A:ARG:C | 1:601:A:SER:N  | 1:601:A:SER:CA | 1:601:A:SER:C | 12       | 1.04          |
| (1,31)  | 2:547:B:SER:N | 2:547:B:SER:CA | 2:547:B:SER:C  | 2:548:B:GLN:N | 11       | 1.04          |
| (1,25)  | 2:544:B:ALA:N | 2:544:B:ALA:CA | 2:544:B:ALA:C  | 2:545:B:LEU:N | 20       | 1.04          |
| (1,22)  | 2:542:B:PHE:C | 2:543:B:SER:N  | 2:543:B:SER:CA | 2:543:B:SER:C | 14       | 1.04          |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 10       | 1.03          |
| (2,85)  | 1:631:A:TYR:C | 1:632:A:ALA:N  | 1:632:A:ALA:CA | 1:632:A:ALA:C | 12       | 1.03          |
| (2,162) | 1:588:A:ARG:N | 1:588:A:ARG:CA | 1:588:A:ARG:C  | 1:589:A:LYS:N | 3        | 1.02          |
| (2,103) | 1:640:A:TYR:C | 1:641:A:GLU:N  | 1:641:A:GLU:CA | 1:641:A:GLU:C | 19       | 1.02          |
| (2,77)  | 1:627:A:ASN:C | 1:628:A:LEU:N  | 1:628:A:LEU:CA | 1:628:A:LEU:C | 5        | 1.02          |
| (2,34)  | 1:605:A:HIS:N | 1:605:A:HIS:CA | 1:605:A:HIS:C  | 1:606:A:LYS:N | 15       | 1.02          |
| (2,31)  | 1:603:A:LEU:C | 1:604:A:VAL:N  | 1:604:A:VAL:CA | 1:604:A:VAL:C | 1        | 1.02          |
| (2,113) | 1:646:A:ARG:C | 1:647:A:ASP:N  | 1:647:A:ASP:CA | 1:647:A:ASP:C | 4        | 1.01          |
| (2,93)  | 1:635:A:VAL:C | 1:636:A:GLU:N  | 1:636:A:GLU:CA | 1:636:A:GLU:C | 13       | 1.01          |
| (1,13)  | 2:538:B:ALA:N | 2:538:B:ALA:CA | 2:538:B:ALA:C  | 2:539:B:ASP:N | 6        | 1.01          |
| (2,162) | 1:588:A:ARG:N | 1:588:A:ARG:CA | 1:588:A:ARG:C  | 1:589:A:LYS:N | 17       | 1.0           |
| (1,30)  | 2:546:B:LEU:C | 2:547:B:SER:N  | 2:547:B:SER:CA | 2:547:B:SER:C | 6        | 1.0           |
| (1,13)  | 2:538:B:ALA:N | 2:538:B:ALA:CA | 2:538:B:ALA:C  | 2:539:B:ASP:N | 12       | 1.0           |