



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 11:31 AM UTC

PDB ID : 7JQ8 / pdb\_00007jq8  
BMRB ID : 30786  
Title : Solution NMR structure of human Brd3 ET domain  
Authors : Aiyer, S.; Swapna, G.V.T.; Roth, J.M.; Montelione, G.T.  
Deposited on : 2020-08-10

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

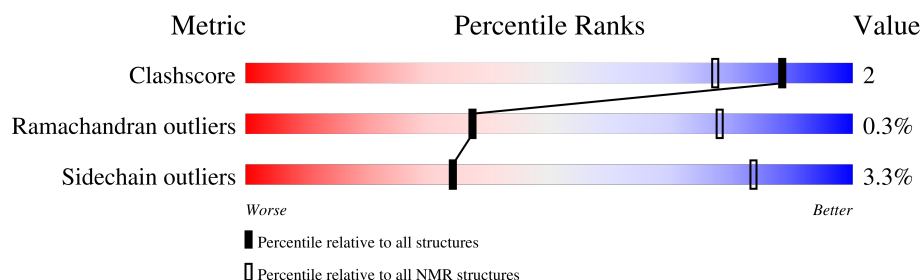
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 79%.

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     | 96     |                  |
| 2   | B     | 23     |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:11-A:23 (13)              | 2.02              | 10           |
| 2                                    | A:26-A:94, B:205-B:221 (86) | 0.88              | 3            |

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

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

The models can be grouped into 5 clusters. No single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1972 atoms, of which 985 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bromodomain-containing protein 3.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 96       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1562  | 484 | 773 | 146 | 156 | 3 |       |

There are 9 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | HIS      | -      | expression tag | UNP Q15059 |
| A     | 2       | HIS      | -      | expression tag | UNP Q15059 |
| A     | 3       | HIS      | -      | expression tag | UNP Q15059 |
| A     | 4       | HIS      | -      | expression tag | UNP Q15059 |
| A     | 5       | HIS      | -      | expression tag | UNP Q15059 |
| A     | 6       | HIS      | -      | expression tag | UNP Q15059 |
| A     | 7       | SER      | -      | expression tag | UNP Q15059 |
| A     | 8       | HIS      | -      | expression tag | UNP Q15059 |
| A     | 9       | MET      | -      | expression tag | UNP Q15059 |

- Molecule 2 is a protein called Integrase peptide.

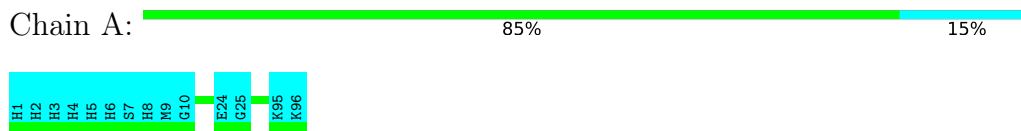
| Mol | Chain | Residues | Atoms |     |     |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|-------|
| 2   | B     | 23       | Total | C   | H   | N  | O  | 0     |
|     |       |          | 410   | 122 | 212 | 43 | 33 |       |

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

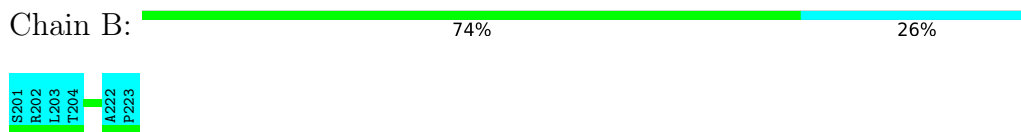
### 4.1 Average score per residue in the NMR ensemble

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: Bromodomain-containing protein 3



- Molecule 2: Integrase peptide

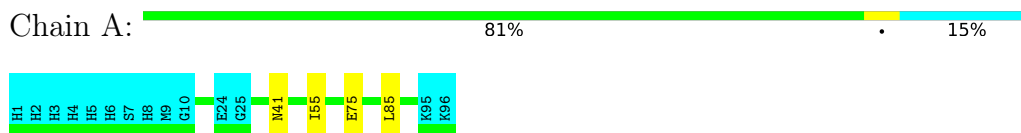


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Bromodomain-containing protein 3

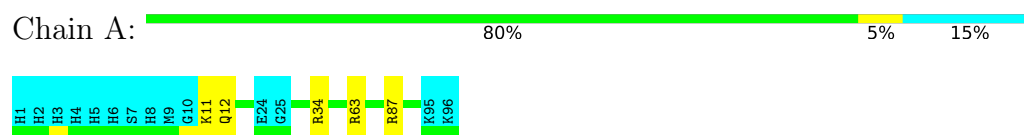


- Molecule 2: Integrase peptide



### 4.2.2 Score per residue for model 2

- Molecule 1: Bromodomain-containing protein 3

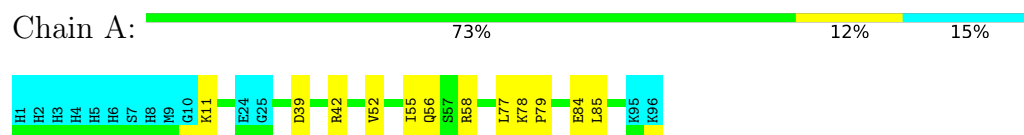


- Molecule 2: Integrase peptide

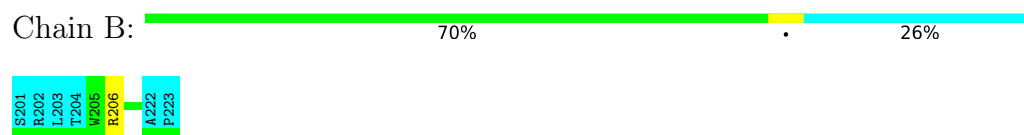


### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Bromodomain-containing protein 3

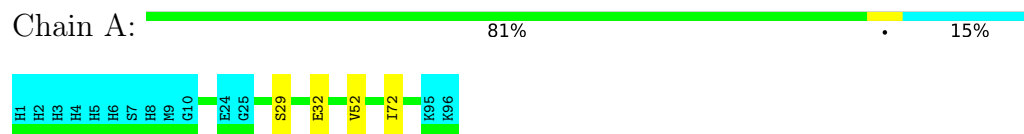


- Molecule 2: Integrase peptide

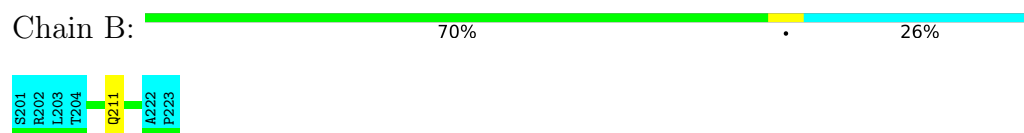


### 4.2.4 Score per residue for model 4

- Molecule 1: Bromodomain-containing protein 3

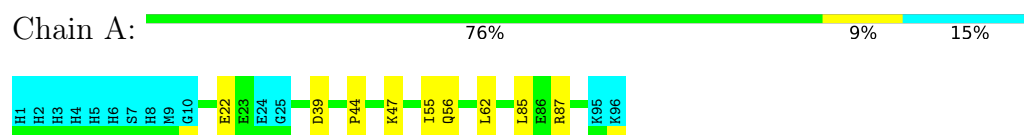


- Molecule 2: Integrase peptide



### 4.2.5 Score per residue for model 5

- Molecule 1: Bromodomain-containing protein 3

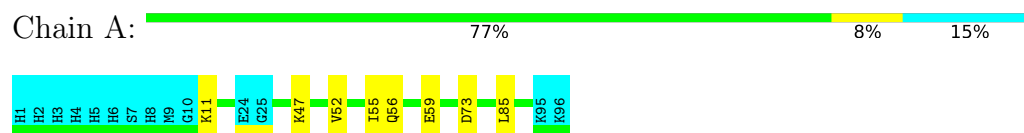


- Molecule 2: Integrase peptide

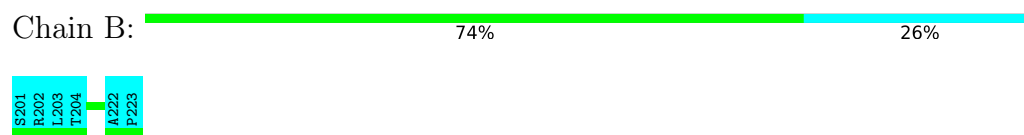


### 4.2.6 Score per residue for model 6

- Molecule 1: Bromodomain-containing protein 3

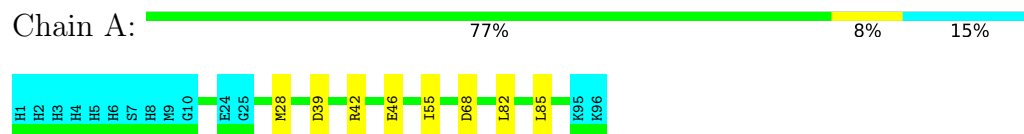


- Molecule 2: Integrase peptide



### 4.2.7 Score per residue for model 7

- Molecule 1: Bromodomain-containing protein 3

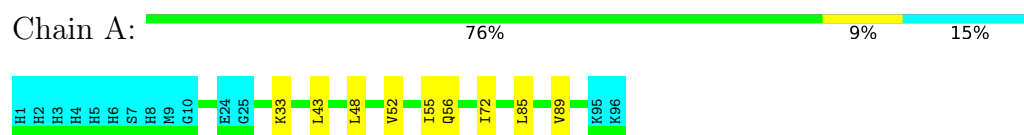


- Molecule 2: Integrase peptide

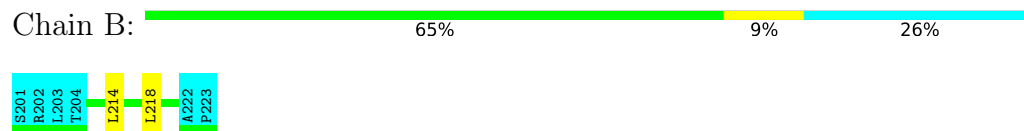


### 4.2.8 Score per residue for model 8

- Molecule 1: Bromodomain-containing protein 3

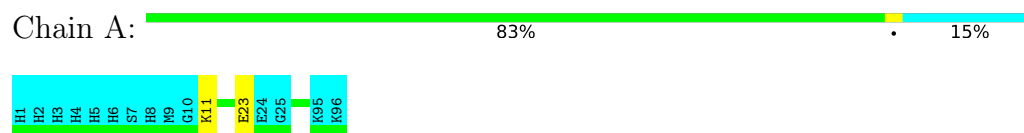


- Molecule 2: Integrase peptide

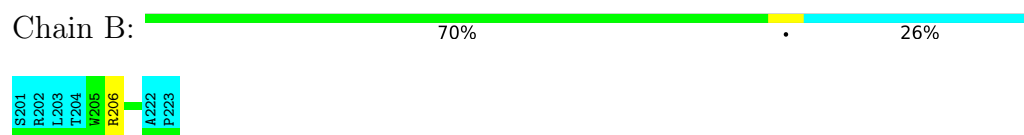


### 4.2.9 Score per residue for model 9

- Molecule 1: Bromodomain-containing protein 3

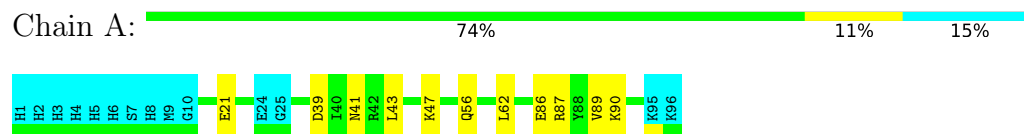


- Molecule 2: Integrase peptide



### 4.2.10 Score per residue for model 10

- Molecule 1: Bromodomain-containing protein 3

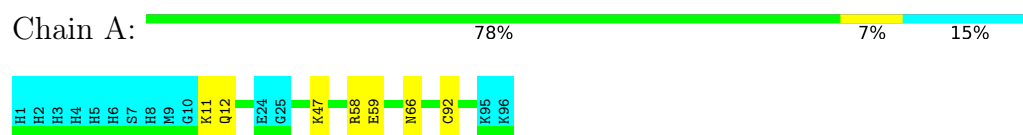


- Molecule 2: Integrase peptide

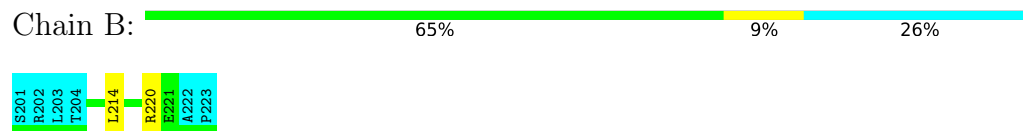


### 4.2.11 Score per residue for model 11

- Molecule 1: Bromodomain-containing protein 3

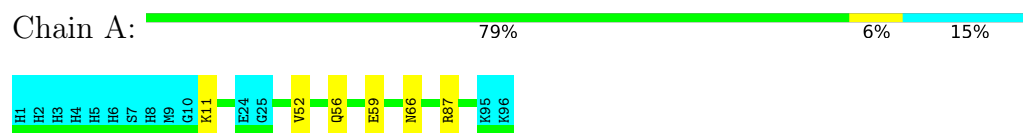


- Molecule 2: Integrase peptide



### 4.2.12 Score per residue for model 12

- Molecule 1: Bromodomain-containing protein 3

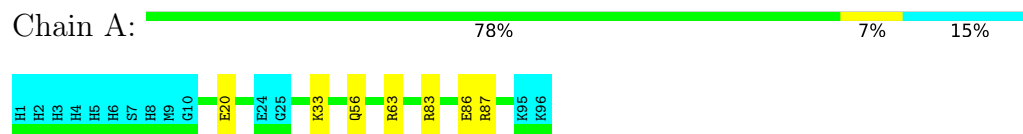


- Molecule 2: Integrase peptide

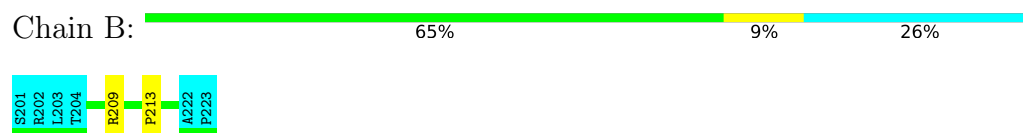


### 4.2.13 Score per residue for model 13

- Molecule 1: Bromodomain-containing protein 3

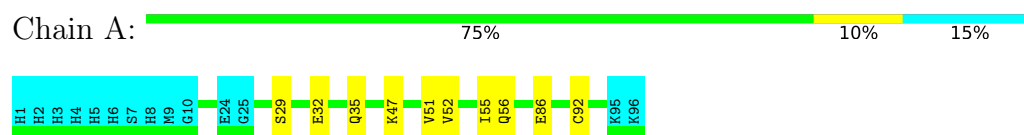


- Molecule 2: Integrase peptide

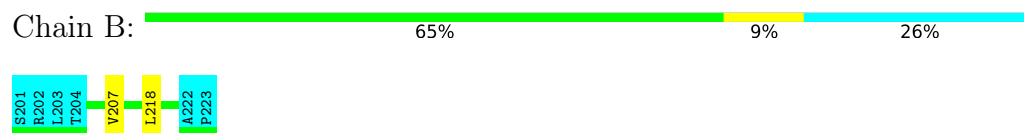


#### 4.2.14 Score per residue for model 14

- Molecule 1: Bromodomain-containing protein 3

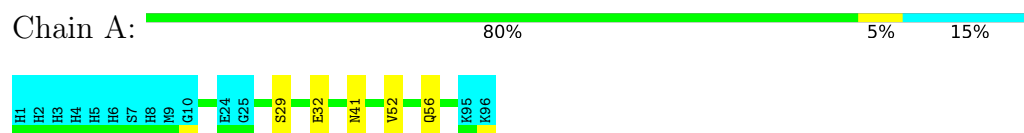


- Molecule 2: Integrase peptide



#### 4.2.15 Score per residue for model 15

- Molecule 1: Bromodomain-containing protein 3

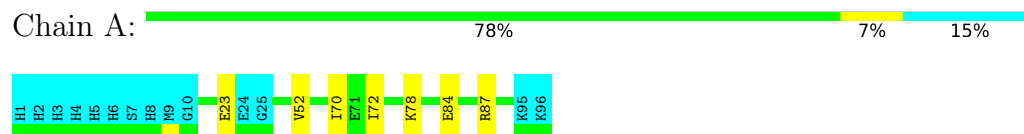


- Molecule 2: Integrase peptide

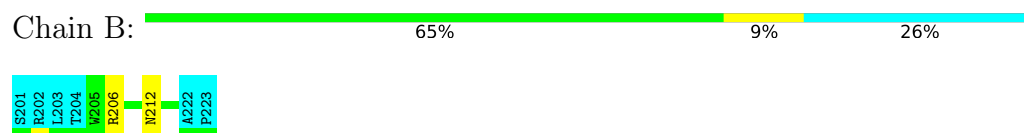


#### 4.2.16 Score per residue for model 16

- Molecule 1: Bromodomain-containing protein 3



- Molecule 2: Integrase peptide



#### 4.2.17 Score per residue for model 17

- Molecule 1: Bromodomain-containing protein 3

Chain A: 



- Molecule 2: Integrase peptide

Chain B: 



#### 4.2.18 Score per residue for model 18

- Molecule 1: Bromodomain-containing protein 3

Chain A: 



- Molecule 2: Integrase peptide

Chain B: 



#### 4.2.19 Score per residue for model 19

- Molecule 1: Bromodomain-containing protein 3

Chain A: 



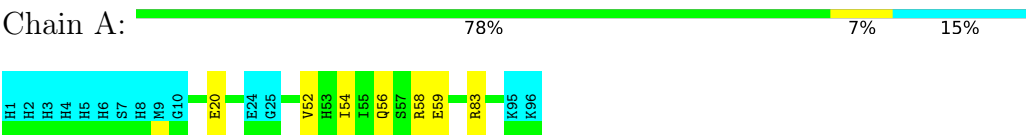
- Molecule 2: Integrase peptide

Chain B: 

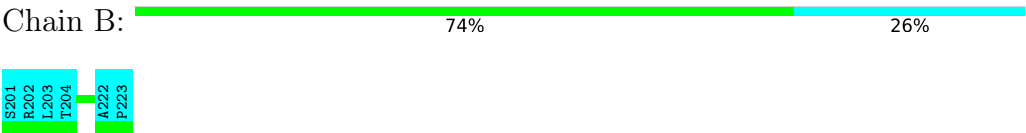


4.2.20 Score per residue for model 20

- Molecule 1: Bromodomain-containing protein 3



- Molecule 2: Integrase peptide



## 5 Refinement protocol and experimental data overview

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

Of the 200 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 |
|---------------|-----------------------|---------|
| CNS           | refinement            |         |
| CYANA         | structure calculation |         |
| ASDP          | geometry optimization | 2.3     |

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                       | 1218           |
| Number of shifts mapped to atoms             | 1218           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 79%            |

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 1.20±0.03    | 0±0/680 ( 0.0± 0.1%) | 1.01±0.03   | 0±0/917 ( 0.0± 0.0%) |
| 2   | B     | 1.18±0.06    | 0±0/156 ( 0.0± 0.1%) | 0.83±0.05   | 0±0/210 ( 0.0± 0.0%) |
| All | All   | 1.19         | 4/16720 ( 0.0%)      | 0.98        | 1/22540 ( 0.0%)      |

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

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 2   | B     | 212 | ASN  | C-N   | 5.79 | 1.38        | 1.33     | 16     | 1     |
| 1   | A     | 66  | ASN  | C-N   | 5.27 | 1.37        | 1.33     | 11     | 2     |
| 1   | A     | 59  | GLU  | C-N   | 5.16 | 1.38        | 1.33     | 12     | 1     |

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|----------|------|-------------|----------|--------|-------|
|     |       |     |      |          |      |             |          | Worst  | Total |
| 1   | A     | 73  | ASP  | CA-CB-CG | 5.65 | 118.25      | 112.60   | 6      | 1     |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 670   | 663      | 662      | 3±2     |
| 2   | B     | 153   | 164      | 164      | 1±1     |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| All | All   | 16460 | 16540    | 16520    | 62      |

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 2.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:47:LYS:HE2   | 1:A:92:CYS:SG    | 0.61     | 2.34        | 11     | 1     |
| 1:A:52:VAL:HG11  | 2:B:218:LEU:HD22 | 0.61     | 1.71        | 18     | 1     |
| 1:A:43:LEU:HD12  | 1:A:47:LYS:HZ2   | 0.58     | 1.57        | 10     | 1     |
| 1:A:56:GLN:HE22  | 1:A:62:LEU:HB2   | 0.57     | 1.58        | 5      | 2     |
| 1:A:29:SER:HB2   | 1:A:32:GLU:HG2   | 0.56     | 1.77        | 14     | 3     |
| 1:A:43:LEU:HD11  | 1:A:89:VAL:HG22  | 0.56     | 1.77        | 19     | 2     |
| 1:A:68:ASP:HB3   | 2:B:220:ARG:HB2  | 0.54     | 1.80        | 7      | 1     |
| 1:A:52:VAL:HG12  | 1:A:72:ILE:HD11  | 0.53     | 1.80        | 18     | 4     |
| 2:B:209:ARG:HD3  | 2:B:213:PRO:HA   | 0.53     | 1.80        | 5      | 1     |
| 2:B:212:ASN:HB2  | 2:B:215:LYS:HG2  | 0.51     | 1.81        | 2      | 1     |
| 2:B:209:ARG:HD2  | 2:B:213:PRO:HA   | 0.50     | 1.82        | 13     | 2     |
| 1:A:55:ILE:HD11  | 1:A:85:LEU:HD11  | 0.50     | 1.84        | 3      | 2     |
| 1:A:48:LEU:HB3   | 2:B:218:LEU:HD21 | 0.49     | 1.84        | 8      | 1     |
| 1:A:56:GLN:HB3   | 1:A:63:ARG:HB2   | 0.48     | 1.84        | 13     | 1     |
| 2:B:207:VAL:HG13 | 2:B:216:ILE:HB   | 0.47     | 1.87        | 12     | 1     |
| 1:A:52:VAL:O     | 1:A:56:GLN:HG2   | 0.46     | 2.10        | 15     | 7     |
| 1:A:83:ARG:HA    | 1:A:86:GLU:HG2   | 0.46     | 1.86        | 13     | 1     |
| 1:A:55:ILE:HD11  | 1:A:85:LEU:HD21  | 0.46     | 1.88        | 8      | 4     |
| 1:A:34:ARG:NH1   | 2:B:213:PRO:HB2  | 0.46     | 2.26        | 2      | 1     |
| 1:A:41:ASN:HA    | 2:B:207:VAL:HG11 | 0.46     | 1.87        | 1      | 2     |
| 2:B:207:VAL:HG22 | 2:B:218:LEU:HG   | 0.45     | 1.89        | 14     | 1     |
| 1:A:43:LEU:HD22  | 1:A:92:CYS:SG    | 0.45     | 2.50        | 18     | 1     |
| 1:A:28:MET:HE3   | 1:A:82:LEU:HB3   | 0.45     | 1.88        | 7      | 1     |
| 1:A:44:PRO:HD2   | 1:A:47:LYS:HD3   | 0.44     | 1.90        | 5      | 1     |
| 1:A:51:VAL:O     | 1:A:55:ILE:HG12  | 0.44     | 2.13        | 19     | 2     |
| 1:A:43:LEU:HD11  | 1:A:89:VAL:HG23  | 0.43     | 1.89        | 18     | 1     |
| 1:A:39:ASP:HB3   | 1:A:89:VAL:HG11  | 0.43     | 1.91        | 10     | 2     |
| 1:A:69:GLU:HG2   | 2:B:219:THR:HG22 | 0.43     | 1.91        | 19     | 1     |
| 2:B:212:ASN:ND2  | 2:B:214:LEU:HB2  | 0.42     | 2.29        | 12     | 1     |
| 1:A:75:GLU:HB3   | 2:B:214:LEU:HD13 | 0.42     | 1.92        | 1      | 1     |
| 1:A:39:ASP:O     | 1:A:42:ARG:HG2   | 0.42     | 2.15        | 7      | 2     |
| 1:A:47:LYS:HG2   | 1:A:92:CYS:SG    | 0.41     | 2.55        | 14     | 1     |
| 1:A:78:LYS:HD2   | 1:A:79:PRO:HD2   | 0.41     | 1.91        | 3      | 1     |
| 1:A:52:VAL:HB    | 1:A:70:ILE:HG21  | 0.41     | 1.93        | 16     | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 2:B:212:ASN:HB2  | 2:B:215:LYS:HG3 | 0.41     | 1.91        | 17     | 1     |
| 1:A:85:LEU:O     | 1:A:89:VAL:HG23 | 0.40     | 2.16        | 19     | 1     |
| 2:B:207:VAL:HG23 | 2:B:216:ILE:HB  | 0.40     | 1.94        | 7      | 1     |
| 1:A:47:LYS:HE3   | 1:A:47:LYS:HA   | 0.40     | 1.94        | 18     | 1     |
| 2:B:212:ASN:HB3  | 2:B:215:LYS:HD3 | 0.40     | 1.93        | 10     | 1     |
| 1:A:54:ILE:O     | 1:A:58:ARG:HD3  | 0.40     | 2.16        | 20     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured     | Allowed     | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|-------------|------------|-------------|----|
| 1   | A     | 82/96 (85%)     | 79±2 (97±2%) | 3±2 (3±2%)  | 0±0 (0±0%) | 49          | 83 |
| 2   | B     | 17/23 (74%)     | 15±1 (89±8%) | 2±1 (10±8%) | 0±0 (1±2%) | 13          | 61 |
| All | All   | 1980/2380 (83%) | 1886 (95%)   | 89 (4%)     | 5 (0%)     | 37          | 78 |

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 211 | GLN  | 4              |
| 1   | A     | 20  | GLU  | 1              |

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

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

| Mol | Chain | Analysed    | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|-------------|--------------|------------|-------------|----|
| 1   | A     | 78/90 (87%) | 76±1 (97±2%) | 2±1 (3±2%) | 36          | 85 |
| 2   | B     | 17/22 (77%) | 16±1 (96±4%) | 1±1 (4±4%) | 28          | 79 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| All | All   | 1900/2240 (85%) | 1837 (97%) | 63 (3%)  | 34 83       |

All 28 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     | 11  | LYS  | 7              |
| 1   | A     | 87  | ARG  | 7              |
| 2   | B     | 206 | ARG  | 6              |
| 2   | B     | 215 | LYS  | 3              |
| 1   | A     | 39  | ASP  | 3              |
| 1   | A     | 59  | GLU  | 3              |
| 1   | A     | 23  | GLU  | 3              |
| 1   | A     | 12  | GLN  | 2              |
| 1   | A     | 58  | ARG  | 2              |
| 1   | A     | 84  | GLU  | 2              |
| 1   | A     | 47  | LYS  | 2              |
| 1   | A     | 33  | LYS  | 2              |
| 2   | B     | 214 | LEU  | 2              |
| 1   | A     | 86  | GLU  | 2              |
| 1   | A     | 90  | LYS  | 2              |
| 2   | B     | 220 | ARG  | 2              |
| 1   | A     | 35  | GLN  | 2              |
| 1   | A     | 63  | ARG  | 1              |
| 1   | A     | 77  | LEU  | 1              |
| 1   | A     | 22  | GLU  | 1              |
| 2   | B     | 219 | THR  | 1              |
| 1   | A     | 46  | GLU  | 1              |
| 1   | A     | 21  | GLU  | 1              |
| 1   | A     | 41  | ASN  | 1              |
| 1   | A     | 78  | LYS  | 1              |
| 1   | A     | 94  | GLN  | 1              |
| 1   | A     | 20  | GLU  | 1              |
| 1   | A     | 83  | ARG  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 71% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1218 |
| Number of shifts mapped to atoms        | 1218 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 1    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 107      | $-0.35 \pm 0.14$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 103      | $0.04 \pm 0.07$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 99       | $0.42 \pm 0.35$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 1133 atoms were assigned a chemical shift out of a possible 1435. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 383/485 (79%) | 193/194 (99%) | 98/198 (49%)    | 92/93 (99%)     |
| Sidechain | 702/893 (79%) | 477/570 (84%) | 216/275 (79%)   | 9/48 (19%)      |

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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 | 48/57 (84%)     | 24/27 (89%)          | 23/27 (85%)           | 1/3 (33%)             |
| Overall  | 1133/1435 (79%) | 694/791 (88%)        | 337/500 (67%)         | 102/144 (71%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 1217 atoms were assigned a chemical shift out of a possible 1711. 0 out of 17 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  | 421/585 (72%)   | 215/235 (91%)        | 107/238 (45%)         | 99/112 (88%)          |
| Sidechain | 748/1013 (74%)  | 511/648 (79%)        | 228/312 (73%)         | 9/53 (17%)            |
| Aromatic  | 48/113 (42%)    | 24/55 (44%)          | 23/41 (56%)           | 1/17 (6%)             |
| Overall   | 1217/1711 (71%) | 750/938 (80%)        | 358/591 (61%)         | 109/182 (60%)         |

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

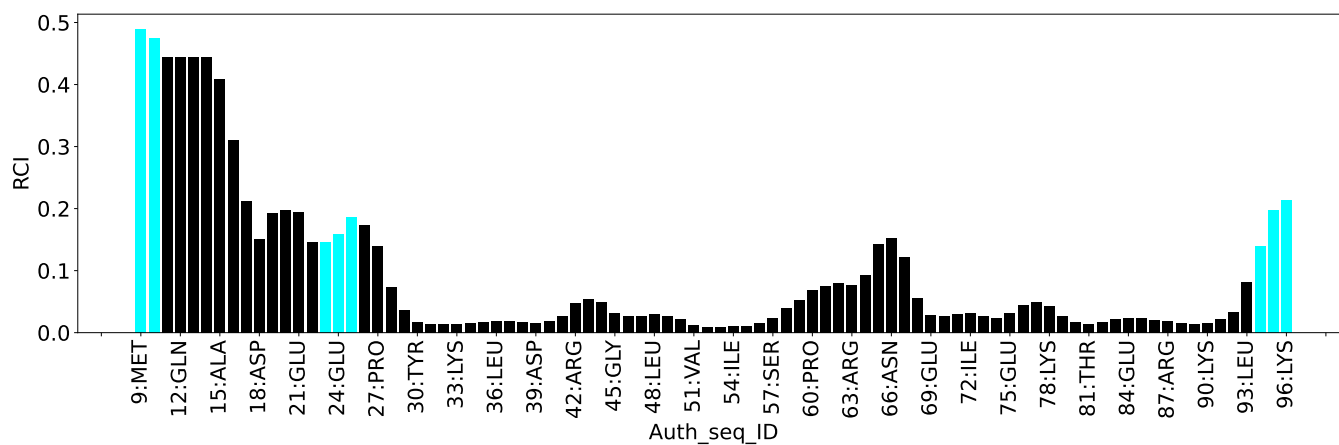
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | B     | 220 | ARG  | HB2  | 0.45       | 0.52 – 3.08         | -5.3    |

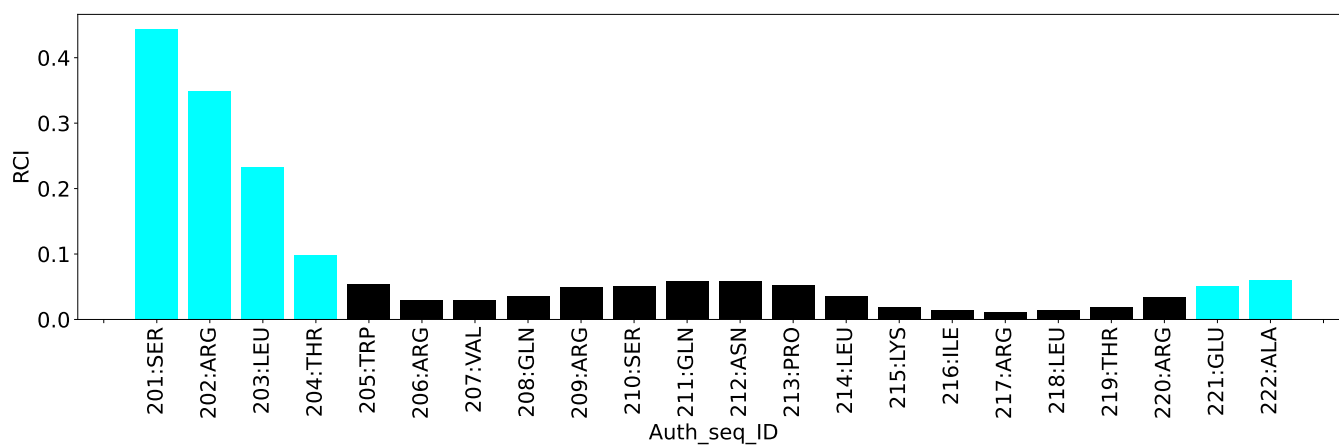
#### 7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



## 8 NMR restraints analysis [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                                | 2255  |
| Intra-residue ( $ i-j =0$ )                              | 563   |
| Sequential ( $ i-j =1$ )                                 | 616   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 430   |
| Long range ( $ i-j \geq 5$ )                             | 389   |
| Inter-chain                                              | 235   |
| Hydrogen bond restraints                                 | 22    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 166   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 20.3  |
| Number of long range restraints per residue <sup>1</sup> | 3.3   |

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations [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)  | 17.4                                   | 0.2     |
| 0.2-0.5 (Medium) | 26.4                                   | 0.5     |
| >0.5 (Large)     | 41.1                                   | 6.16    |

### 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)   | 13.1                                   | 9.92    |
| 10.0-20.0 (Medium) | 3.1                                    | 19.91   |
| >20.0 (Large)      | 2.0                                    | 113.51  |

## 9 Distance violation analysis ⓘ

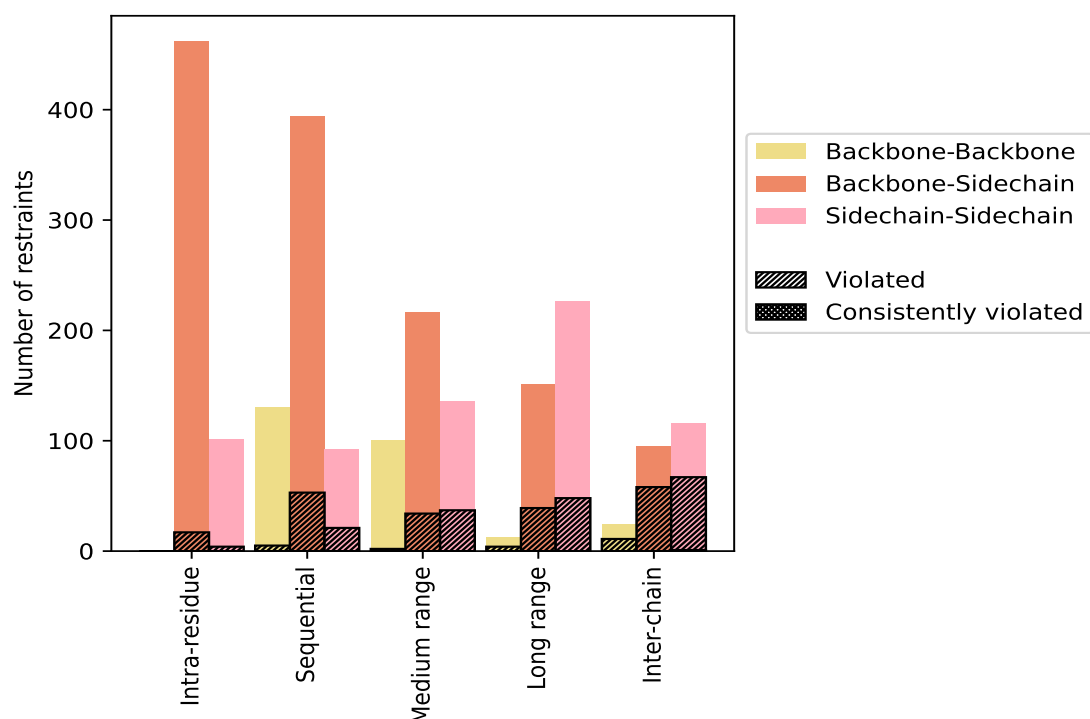
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                             | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                     |                     |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|---------------------|---------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>      | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">563</a>  | <a href="#">25.0</a>  | <a href="#">21</a>    | <a href="#">3.7</a>  | <a href="#">0.9</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 462                  | 20.5                  | 17                    | 3.7                  | 0.8                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 101                  | 4.5                   | 4                     | 4.0                  | 0.2                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">616</a>  | <a href="#">27.3</a>  | <a href="#">79</a>    | <a href="#">12.8</a> | <a href="#">3.5</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 130                  | 5.8                   | 5                     | 3.8                  | 0.2                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 394                  | 17.5                  | 53                    | 13.5                 | 2.4                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 92                   | 4.1                   | 21                    | 22.8                 | 0.9                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">430</a>  | <a href="#">19.1</a>  | <a href="#">54</a>    | <a href="#">12.6</a> | <a href="#">2.4</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 100                  | 4.4                   | 2                     | 2.0                  | 0.1                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 194                  | 8.6                   | 15                    | 7.7                  | 0.7                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 136                  | 6.0                   | 37                    | 27.2                 | 1.6                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">389</a>  | <a href="#">17.3</a>  | <a href="#">91</a>    | <a href="#">23.4</a> | <a href="#">4.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 12                   | 0.5                   | 4                     | 33.3                 | 0.2                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 151                  | 6.7                   | 39                    | 25.8                 | 1.7                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 226                  | 10.0                  | 48                    | 21.2                 | 2.1                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Inter-chain</a>                                | <a href="#">235</a>  | <a href="#">10.4</a>  | <a href="#">136</a>   | <a href="#">57.9</a> | <a href="#">6.0</a>  | <a href="#">1</a>                  | <a href="#">0.4</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 24                   | 1.1                   | 11                    | 45.8                 | 0.5                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 95                   | 4.2                   | 58                    | 61.1                 | 2.6                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 116                  | 5.1                   | 67                    | 57.8                 | 3.0                  | 1                                  | 0.9                 | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">22</a>   | <a href="#">1.0</a>   | <a href="#">19</a>    | <a href="#">86.4</a> | <a href="#">0.8</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">2255</a> | <a href="#">100.0</a> | <a href="#">400</a>   | <a href="#">17.7</a> | <a href="#">17.7</a> | <a href="#">1</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 266                  | 11.8                  | 22                    | 8.3                  | 1.0                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 1318                 | 58.4                  | 201                   | 15.3                 | 8.9                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 671                  | 29.8                  | 177                   | 26.4                 | 7.8                  | 1                                  | 0.1                 | 0.0                 |

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and 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        | 1                    | 17              | 14              | 23              | 21              | 76    | 0.58     | 1.72    | 0.4                 | 0.52       |
| 2        | 4                    | 14              | 21              | 29              | 29              | 97    | 0.82     | 2.75    | 0.67                | 0.58       |
| 3        | 1                    | 20              | 17              | 24              | 42              | 104   | 1.32     | 5.72    | 1.46                | 0.66       |
| 4        | 0                    | 18              | 13              | 23              | 36              | 90    | 1.35     | 6.16    | 1.53                | 0.59       |
| 5        | 0                    | 14              | 9               | 17              | 22              | 62    | 0.47     | 1.98    | 0.41                | 0.33       |
| 6        | 1                    | 14              | 16              | 20              | 22              | 73    | 0.68     | 2.39    | 0.5                 | 0.56       |
| 7        | 1                    | 14              | 23              | 9               | 20              | 67    | 0.4      | 1.74    | 0.35                | 0.28       |
| 8        | 2                    | 19              | 12              | 27              | 38              | 98    | 0.99     | 4.86    | 1.06                | 0.56       |
| 9        | 2                    | 21              | 21              | 18              | 39              | 101   | 0.76     | 2.81    | 0.67                | 0.5        |
| 10       | 2                    | 12              | 16              | 15              | 20              | 65    | 0.66     | 2.96    | 0.66                | 0.38       |

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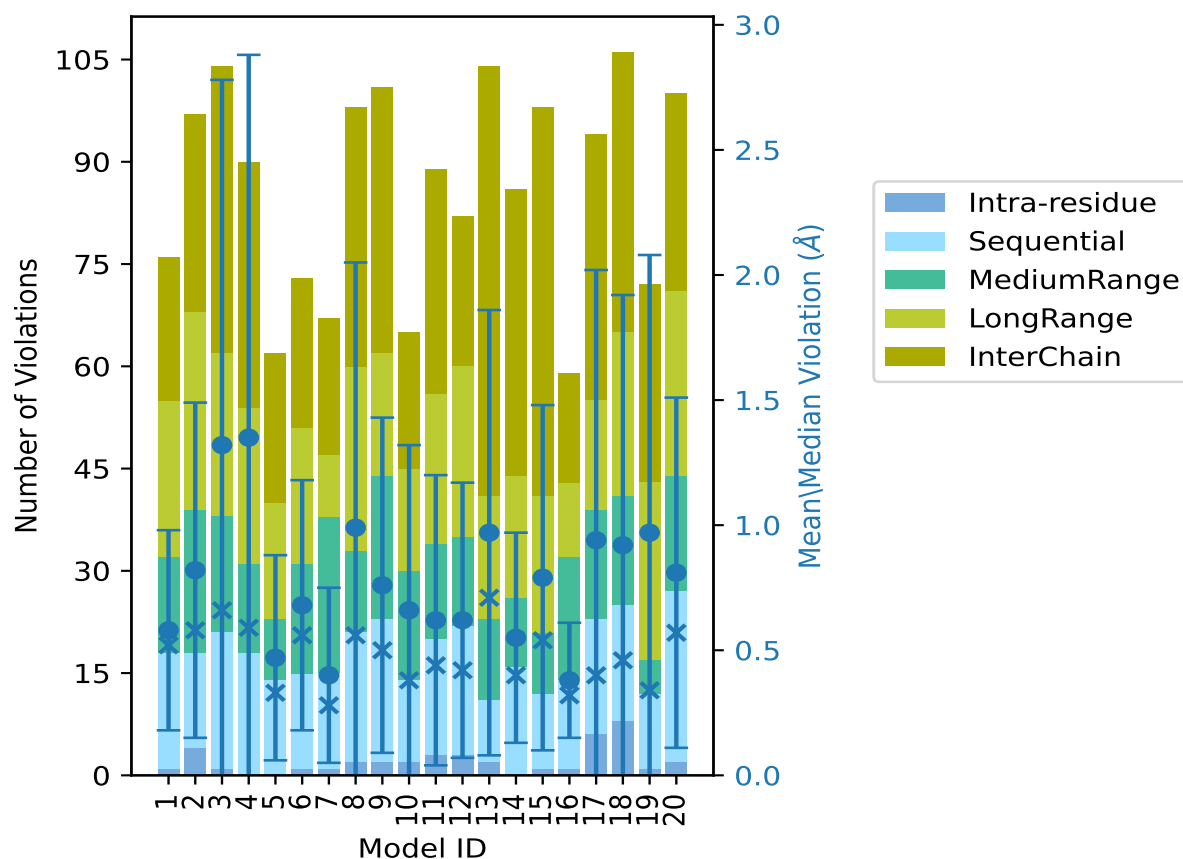
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 3                    | 17              | 14              | 22              | 33              | 89    | 0.62     | 2.85    | 0.58                | 0.44       |
| 12       | 3                    | 19              | 13              | 25              | 22              | 82    | 0.62     | 2.77    | 0.55                | 0.42       |
| 13       | 2                    | 9               | 12              | 18              | 63              | 104   | 0.97     | 4.75    | 0.89                | 0.71       |
| 14       | 0                    | 16              | 10              | 18              | 42              | 86    | 0.55     | 1.91    | 0.42                | 0.4        |
| 15       | 1                    | 11              | 9               | 20              | 57              | 98    | 0.79     | 3.15    | 0.69                | 0.54       |
| 16       | 1                    | 13              | 18              | 11              | 16              | 59    | 0.38     | 0.94    | 0.23                | 0.32       |
| 17       | 6                    | 17              | 16              | 16              | 39              | 94    | 0.94     | 5.2     | 1.08                | 0.4        |
| 18       | 8                    | 17              | 16              | 24              | 41              | 106   | 0.92     | 4.38    | 1.0                 | 0.46       |
| 19       | 1                    | 11              | 5               | 26              | 29              | 72    | 0.97     | 4.39    | 1.11                | 0.34       |
| 20       | 2                    | 25              | 17              | 27              | 29              | 100   | 0.81     | 3.18    | 0.7                 | 0.57       |

<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

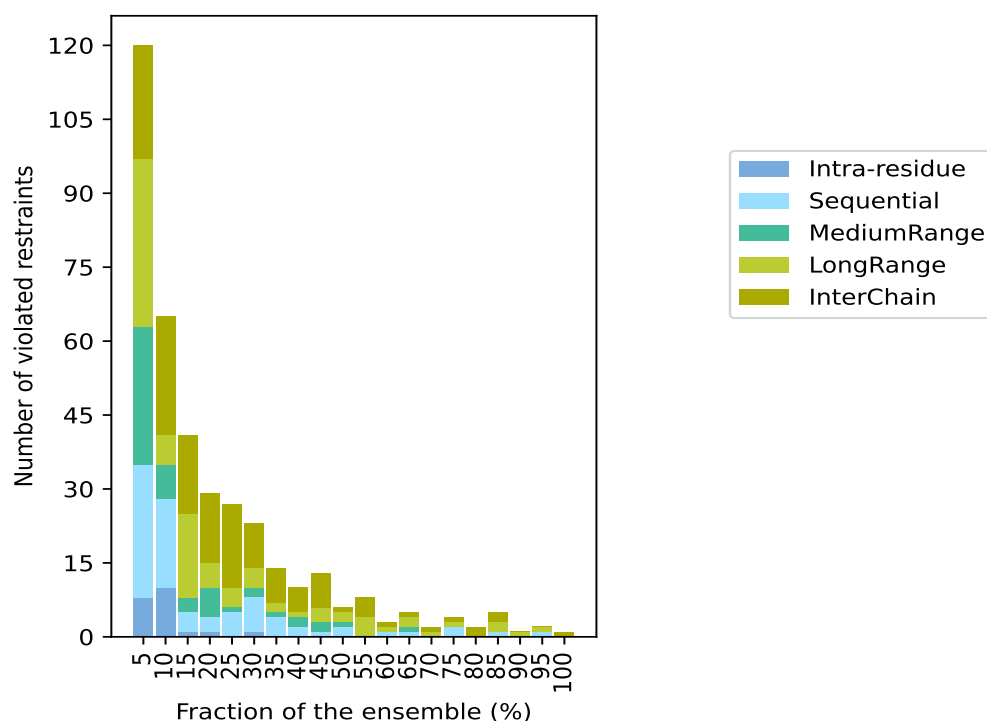
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1852(IR:542, SQ:537, MR:376, LR:298, IC:99) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 8                             | 27              | 28              | 34              | 23              | 120   | 1                        | 5.0   |
| 10                            | 18              | 7               | 6               | 24              | 65    | 2                        | 10.0  |
| 1                             | 4               | 3               | 17              | 16              | 41    | 3                        | 15.0  |
| 1                             | 3               | 6               | 5               | 14              | 29    | 4                        | 20.0  |
| 0                             | 5               | 1               | 4               | 17              | 27    | 5                        | 25.0  |
| 1                             | 7               | 2               | 4               | 9               | 23    | 6                        | 30.0  |
| 0                             | 4               | 1               | 2               | 7               | 14    | 7                        | 35.0  |
| 0                             | 2               | 2               | 1               | 5               | 10    | 8                        | 40.0  |
| 0                             | 1               | 2               | 3               | 7               | 13    | 9                        | 45.0  |
| 0                             | 2               | 1               | 2               | 1               | 6     | 10                       | 50.0  |
| 0                             | 0               | 0               | 4               | 4               | 8     | 11                       | 55.0  |
| 0                             | 1               | 0               | 1               | 1               | 3     | 12                       | 60.0  |
| 0                             | 1               | 1               | 2               | 1               | 5     | 13                       | 65.0  |
| 0                             | 0               | 0               | 1               | 1               | 2     | 14                       | 70.0  |
| 0                             | 2               | 0               | 1               | 1               | 4     | 15                       | 75.0  |
| 0                             | 0               | 0               | 0               | 2               | 2     | 16                       | 80.0  |
| 0                             | 1               | 0               | 2               | 2               | 5     | 17                       | 85.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 18                       | 90.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 19                       | 95.0  |
| 0                             | 0               | 0               | 0               | 1               | 1     | 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

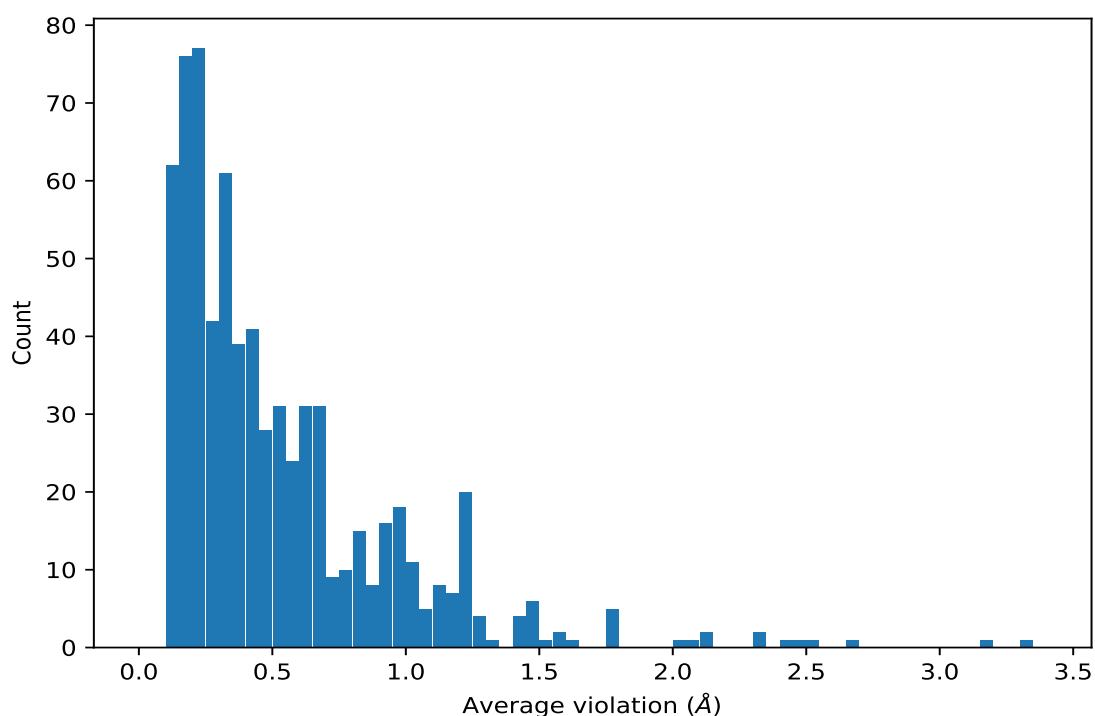
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,58)   | 1:76:A:THR:HG21 | 2:215:B:LYS:HG3 | 20                  | 1.42     | 0.7                 | 1.38       |
| (2,58)   | 1:76:A:THR:HG22 | 2:215:B:LYS:HG3 | 20                  | 1.42     | 0.7                 | 1.38       |
| (2,58)   | 1:76:A:THR:HG23 | 2:215:B:LYS:HG3 | 20                  | 1.42     | 0.7                 | 1.38       |
| (2,1144) | 2:205:B:TRP:HZ3 | 2:219:B:THR:HA  | 19                  | 2.51     | 1.21                | 2.54       |
| (2,12)   | 2:204:B:THR:HB  | 2:205:B:TRP:HD1 | 19                  | 1.13     | 0.82                | 0.85       |
| (2,1251) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HG  | 18                  | 2.12     | 1.47                | 2.1        |
| (2,1340) | 2:205:B:TRP:HE3 | 2:219:B:THR:H   | 17                  | 1.75     | 1.02                | 1.9        |
| (2,1145) | 2:205:B:TRP:HE3 | 2:219:B:THR:HA  | 17                  | 1.46     | 0.87                | 1.5        |
| (2,1474) | 1:75:A:GLU:HG2  | 2:215:B:LYS:H   | 17                  | 0.83     | 0.4                 | 0.79       |
| (2,1293) | 1:69:A:GLU:HG3  | 2:219:B:THR:HB  | 17                  | 0.71     | 0.59                | 0.37       |
| (2,1265) | 2:204:B:THR:HB  | 2:205:B:TRP:HB3 | 17                  | 0.71     | 0.22                | 0.77       |
| (1,13)   | 1:51:A:VAL:O    | 1:55:A:ILE:N    | 17                  | 0.55     | 0.24                | 0.6        |
| (2,28)   | 1:69:A:GLU:HA   | 2:205:B:TRP:HZ3 | 16                  | 3.17     | 1.8                 | 2.89       |
| (2,189)  | 1:70:A:ILE:HG12 | 2:205:B:TRP:HH2 | 16                  | 2.05     | 1.62                | 2.01       |
| (1,14)   | 1:51:A:VAL:O    | 1:55:A:ILE:H    | 16                  | 0.52     | 0.23                | 0.55       |
| (2,531)  | 1:76:A:THR:HG21 | 2:215:B:LYS:HD3 | 15                  | 1.15     | 0.93                | 0.73       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,531)  | 1:76:A:THR:HG22  | 2:215:B:LYS:HD3  | 15                  | 1.15     | 0.93                | 0.73       |
| (2,531)  | 1:76:A:THR:HG23  | 2:215:B:LYS:HD3  | 15                  | 1.15     | 0.93                | 0.73       |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H    | 15                  | 0.98     | 0.53                | 1.19       |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 15                  | 0.5      | 0.12                | 0.49       |
| (2,1386) | 2:204:B:THR:HB   | 2:205:B:TRP:H    | 15                  | 0.38     | 0.16                | 0.45       |
| (2,991)  | 1:70:A:ILE:H     | 2:205:B:TRP:HZ3  | 14                  | 3.32     | 1.68                | 3.58       |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG   | 14                  | 0.71     | 0.5                 | 0.57       |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 14                  | 0.43     | 0.16                | 0.46       |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H     | 14                  | 0.3      | 0.13                | 0.26       |
| (2,1127) | 1:70:A:ILE:H     | 2:205:B:TRP:HH2  | 13                  | 2.04     | 1.37                | 2.28       |
| (2,1231) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HA   | 13                  | 1.61     | 0.67                | 1.55       |
| (2,1163) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HB3  | 13                  | 1.56     | 0.97                | 1.45       |
| (2,11)   | 2:204:B:THR:HA   | 2:205:B:TRP:HD1  | 13                  | 1.07     | 0.5                 | 0.82       |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 13                  | 0.79     | 0.52                | 0.59       |
| (2,16)   | 2:205:B:TRP:HZ3  | 2:218:B:LEU:HB3  | 12                  | 1.76     | 0.85                | 1.5        |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB2  | 12                  | 0.8      | 0.59                | 0.57       |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB3  | 12                  | 0.8      | 0.59                | 0.57       |
| (1,12)   | 1:50:A:ARG:O     | 1:54:A:ILE:H     | 12                  | 0.38     | 0.13                | 0.38       |
| (2,2222) | 2:218:B:LEU:HD11 | 2:219:B:THR:H    | 12                  | 0.3      | 0.04                | 0.3        |
| (2,2222) | 2:218:B:LEU:HD12 | 2:219:B:THR:H    | 12                  | 0.3      | 0.04                | 0.3        |
| (2,2222) | 2:218:B:LEU:HD13 | 2:219:B:THR:H    | 12                  | 0.3      | 0.04                | 0.3        |
| (2,2222) | 2:218:B:LEU:HD21 | 2:219:B:THR:H    | 12                  | 0.3      | 0.04                | 0.3        |
| (2,2222) | 2:218:B:LEU:HD22 | 2:219:B:THR:H    | 12                  | 0.3      | 0.04                | 0.3        |
| (2,2222) | 2:218:B:LEU:HD23 | 2:219:B:THR:H    | 12                  | 0.3      | 0.04                | 0.3        |
| (2,13)   | 1:70:A:ILE:HG12  | 2:205:B:TRP:HZ3  | 11                  | 2.65     | 1.31                | 2.89       |
| (2,650)  | 1:70:A:ILE:HB    | 2:205:B:TRP:HZ3  | 11                  | 2.48     | 1.23                | 2.54       |
| (2,990)  | 1:69:A:GLU:H     | 2:205:B:TRP:HZ3  | 11                  | 2.4      | 1.32                | 2.81       |
| (2,143)  | 1:70:A:ILE:HG13  | 2:205:B:TRP:HH2  | 11                  | 2.32     | 1.26                | 2.13       |
| (2,2149) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG2  | 11                  | 1.47     | 0.64                | 1.54       |
| (2,2149) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG2  | 11                  | 1.47     | 0.64                | 1.54       |
| (2,3)    | 2:205:B:TRP:HE3  | 2:218:B:LEU:HB3  | 11                  | 1.26     | 0.71                | 0.85       |
| (2,2150) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG3  | 11                  | 1.23     | 0.58                | 1.14       |
| (2,2150) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG3  | 11                  | 1.23     | 0.58                | 1.14       |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD11 | 11                  | 0.44     | 0.16                | 0.41       |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD12 | 11                  | 0.44     | 0.16                | 0.41       |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD13 | 11                  | 0.44     | 0.16                | 0.41       |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD21 | 11                  | 0.44     | 0.16                | 0.41       |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD22 | 11                  | 0.44     | 0.16                | 0.41       |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD23 | 11                  | 0.44     | 0.16                | 0.41       |
| (2,208)  | 1:69:A:GLU:HA    | 2:205:B:TRP:HE3  | 10                  | 2.12     | 0.92                | 2.25       |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 10                  | 1.25     | 0.61                | 0.97       |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 10                  | 1.25     | 0.61                | 0.97       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 10                  | 1.25     | 0.61                | 0.97       |
| (2,1479) | 2:208:B:GLN:HE21 | 2:219:B:THR:HB   | 10                  | 0.98     | 0.31                | 1.02       |
| (2,2148) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HB3  | 10                  | 0.68     | 0.46                | 0.6        |
| (2,2148) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HB3  | 10                  | 0.68     | 0.46                | 0.6        |
| (2,2199) | 2:214:B:LEU:HD11 | 2:215:B:LYS:H    | 10                  | 0.3      | 0.16                | 0.24       |
| (2,2199) | 2:214:B:LEU:HD12 | 2:215:B:LYS:H    | 10                  | 0.3      | 0.16                | 0.24       |
| (2,2199) | 2:214:B:LEU:HD13 | 2:215:B:LYS:H    | 10                  | 0.3      | 0.16                | 0.24       |
| (2,2199) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H    | 10                  | 0.3      | 0.16                | 0.24       |
| (2,2199) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H    | 10                  | 0.3      | 0.16                | 0.24       |
| (2,2199) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H    | 10                  | 0.3      | 0.16                | 0.24       |
| (1,21)   | 1:87:A:ARG:O     | 1:91:A:SER:N     | 10                  | 0.29     | 0.19                | 0.22       |
| (1,9)    | 1:49:A:GLY:O     | 1:53:A:HIS:N     | 10                  | 0.25     | 0.1                 | 0.24       |
| (2,1619) | 1:35:A:GLN:HE21  | 1:38:A:LEU:HD11  | 10                  | 0.17     | 0.04                | 0.16       |
| (2,1619) | 1:35:A:GLN:HE21  | 1:38:A:LEU:HD12  | 10                  | 0.17     | 0.04                | 0.16       |
| (2,1619) | 1:35:A:GLN:HE21  | 1:38:A:LEU:HD13  | 10                  | 0.17     | 0.04                | 0.16       |
| (2,1619) | 1:35:A:GLN:HE21  | 1:38:A:LEU:HD21  | 10                  | 0.17     | 0.04                | 0.16       |
| (2,1619) | 1:35:A:GLN:HE21  | 1:38:A:LEU:HD22  | 10                  | 0.17     | 0.04                | 0.16       |
| (2,1619) | 1:35:A:GLN:HE21  | 1:38:A:LEU:HD23  | 10                  | 0.17     | 0.04                | 0.16       |
| (2,1619) | 1:35:A:GLN:HE22  | 1:38:A:LEU:HD11  | 10                  | 0.17     | 0.04                | 0.16       |
| (2,1619) | 1:35:A:GLN:HE22  | 1:38:A:LEU:HD12  | 10                  | 0.17     | 0.04                | 0.16       |
| (2,1619) | 1:35:A:GLN:HE22  | 1:38:A:LEU:HD13  | 10                  | 0.17     | 0.04                | 0.16       |
| (2,1619) | 1:35:A:GLN:HE22  | 1:38:A:LEU:HD21  | 10                  | 0.17     | 0.04                | 0.16       |
| (2,1619) | 1:35:A:GLN:HE22  | 1:38:A:LEU:HD22  | 10                  | 0.17     | 0.04                | 0.16       |
| (2,1619) | 1:35:A:GLN:HE22  | 1:38:A:LEU:HD23  | 10                  | 0.17     | 0.04                | 0.16       |
| (2,15)   | 1:70:A:ILE:HG13  | 2:205:B:TRP:HZ3  | 9                   | 2.34     | 1.03                | 2.21       |
| (2,162)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ3  | 9                   | 1.46     | 0.89                | 1.27       |
| (2,162)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ3  | 9                   | 1.46     | 0.89                | 1.27       |
| (2,162)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ3  | 9                   | 1.46     | 0.89                | 1.27       |
| (2,1606) | 1:34:A:ARG:HD2   | 2:213:B:PRO:HG3  | 9                   | 1.23     | 0.74                | 1.14       |
| (2,1606) | 1:34:A:ARG:HD3   | 2:213:B:PRO:HG3  | 9                   | 1.23     | 0.74                | 1.14       |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD2  | 9                   | 1.2      | 0.53                | 1.21       |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD3  | 9                   | 1.2      | 0.53                | 1.21       |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD2  | 9                   | 1.2      | 0.53                | 1.21       |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD3  | 9                   | 1.2      | 0.53                | 1.21       |
| (2,1931) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG3  | 9                   | 0.97     | 0.39                | 1.15       |
| (2,1931) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG3  | 9                   | 0.97     | 0.39                | 1.15       |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD11 | 9                   | 0.91     | 0.65                | 0.81       |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD12 | 9                   | 0.91     | 0.65                | 0.81       |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD13 | 9                   | 0.91     | 0.65                | 0.81       |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD21 | 9                   | 0.91     | 0.65                | 0.81       |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD22 | 9                   | 0.91     | 0.65                | 0.81       |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD23 | 9                   | 0.91     | 0.65                | 0.81       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD11 | 9                   | 0.65     | 0.34                | 0.61       |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD12 | 9                   | 0.65     | 0.34                | 0.61       |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD13 | 9                   | 0.65     | 0.34                | 0.61       |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD21 | 9                   | 0.65     | 0.34                | 0.61       |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD22 | 9                   | 0.65     | 0.34                | 0.61       |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD23 | 9                   | 0.65     | 0.34                | 0.61       |
| (2,2112) | 2:206:B:ARG:HD2  | 2:207:B:VAL:H    | 9                   | 0.59     | 0.41                | 0.49       |
| (2,2112) | 2:206:B:ARG:HD3  | 2:207:B:VAL:H    | 9                   | 0.59     | 0.41                | 0.49       |
| (2,1237) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB2  | 9                   | 0.58     | 0.53                | 0.36       |
| (2,1475) | 1:73:A:ASP:HA    | 2:216:B:ILE:H    | 9                   | 0.54     | 0.39                | 0.3        |
| (2,2127) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HG   | 9                   | 0.48     | 0.44                | 0.31       |
| (2,2127) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HG   | 9                   | 0.48     | 0.44                | 0.31       |
| (2,2127) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HG   | 9                   | 0.48     | 0.44                | 0.31       |
| (2,2127) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HG   | 9                   | 0.48     | 0.44                | 0.31       |
| (2,2127) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HG   | 9                   | 0.48     | 0.44                | 0.31       |
| (2,2127) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HG   | 9                   | 0.48     | 0.44                | 0.31       |
| (2,1737) | 1:48:A:LEU:HD11  | 2:205:B:TRP:HZ2  | 9                   | 0.42     | 0.21                | 0.39       |
| (2,1737) | 1:48:A:LEU:HD12  | 2:205:B:TRP:HZ2  | 9                   | 0.42     | 0.21                | 0.39       |
| (2,1737) | 1:48:A:LEU:HD13  | 2:205:B:TRP:HZ2  | 9                   | 0.42     | 0.21                | 0.39       |
| (2,1737) | 1:48:A:LEU:HD21  | 2:205:B:TRP:HZ2  | 9                   | 0.42     | 0.21                | 0.39       |
| (2,1737) | 1:48:A:LEU:HD22  | 2:205:B:TRP:HZ2  | 9                   | 0.42     | 0.21                | 0.39       |
| (2,1737) | 1:48:A:LEU:HD23  | 2:205:B:TRP:HZ2  | 9                   | 0.42     | 0.21                | 0.39       |
| (1,18)   | 1:53:A:HIS:O     | 1:57:A:SER:H     | 9                   | 0.39     | 0.23                | 0.31       |
| (2,1621) | 1:35:A:GLN:HE21  | 1:39:A:ASP:HB2   | 9                   | 0.16     | 0.04                | 0.15       |
| (2,1621) | 1:35:A:GLN:HE21  | 1:39:A:ASP:HB3   | 9                   | 0.16     | 0.04                | 0.15       |
| (2,1621) | 1:35:A:GLN:HE22  | 1:39:A:ASP:HB2   | 9                   | 0.16     | 0.04                | 0.15       |
| (2,1621) | 1:35:A:GLN:HE22  | 1:39:A:ASP:HB3   | 9                   | 0.16     | 0.04                | 0.15       |
| (2,100)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HH2  | 8                   | 1.77     | 0.98                | 1.65       |
| (2,100)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HH2  | 8                   | 1.77     | 0.98                | 1.65       |
| (2,100)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HH2  | 8                   | 1.77     | 0.98                | 1.65       |
| (2,1334) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HG3  | 8                   | 1.53     | 0.68                | 1.47       |
| (2,1126) | 1:70:A:ILE:H     | 2:205:B:TRP:HE3  | 8                   | 1.41     | 0.55                | 1.27       |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE2  | 8                   | 1.01     | 0.37                | 1.0        |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE3  | 8                   | 1.01     | 0.37                | 1.0        |
| (2,1407) | 2:213:B:PRO:HG2  | 2:214:B:LEU:H    | 8                   | 0.71     | 0.4                 | 0.54       |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD11 | 8                   | 0.65     | 0.34                | 0.69       |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD12 | 8                   | 0.65     | 0.34                | 0.69       |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD13 | 8                   | 0.65     | 0.34                | 0.69       |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD21 | 8                   | 0.65     | 0.34                | 0.69       |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD22 | 8                   | 0.65     | 0.34                | 0.69       |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD23 | 8                   | 0.65     | 0.34                | 0.69       |
| (2,1250) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HG   | 8                   | 0.57     | 0.34                | 0.52       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1250) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HG   | 8                   | 0.57     | 0.34                | 0.52       |
| (1,17)   | 1:53:A:HIS:O     | 1:57:A:SER:N     | 8                   | 0.43     | 0.22                | 0.34       |
| (1,22)   | 1:87:A:ARG:O     | 1:91:A:SER:H     | 8                   | 0.31     | 0.21                | 0.19       |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD21  | 8                   | 0.15     | 0.02                | 0.15       |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD22  | 8                   | 0.15     | 0.02                | 0.15       |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD23  | 8                   | 0.15     | 0.02                | 0.15       |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD21  | 8                   | 0.15     | 0.02                | 0.15       |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD22  | 8                   | 0.15     | 0.02                | 0.15       |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD23  | 8                   | 0.15     | 0.02                | 0.15       |
| (2,553)  | 1:27:A:PRO:HA    | 1:79:A:PRO:HB3   | 8                   | 0.15     | 0.03                | 0.15       |
| (2,1526) | 1:26:A:LEU:HD11  | 1:27:A:PRO:HG2   | 8                   | 0.12     | 0.01                | 0.12       |
| (2,1526) | 1:26:A:LEU:HD11  | 1:27:A:PRO:HG3   | 8                   | 0.12     | 0.01                | 0.12       |
| (2,1526) | 1:26:A:LEU:HD12  | 1:27:A:PRO:HG2   | 8                   | 0.12     | 0.01                | 0.12       |
| (2,1526) | 1:26:A:LEU:HD12  | 1:27:A:PRO:HG3   | 8                   | 0.12     | 0.01                | 0.12       |
| (2,1526) | 1:26:A:LEU:HD13  | 1:27:A:PRO:HG2   | 8                   | 0.12     | 0.01                | 0.12       |
| (2,1526) | 1:26:A:LEU:HD13  | 1:27:A:PRO:HG3   | 8                   | 0.12     | 0.01                | 0.12       |
| (2,1526) | 1:26:A:LEU:HD21  | 1:27:A:PRO:HG2   | 8                   | 0.12     | 0.01                | 0.12       |
| (2,1526) | 1:26:A:LEU:HD21  | 1:27:A:PRO:HG3   | 8                   | 0.12     | 0.01                | 0.12       |
| (2,1526) | 1:26:A:LEU:HD22  | 1:27:A:PRO:HG2   | 8                   | 0.12     | 0.01                | 0.12       |
| (2,1526) | 1:26:A:LEU:HD22  | 1:27:A:PRO:HG3   | 8                   | 0.12     | 0.01                | 0.12       |
| (2,1526) | 1:26:A:LEU:HD23  | 1:27:A:PRO:HG2   | 8                   | 0.12     | 0.01                | 0.12       |
| (2,1526) | 1:26:A:LEU:HD23  | 1:27:A:PRO:HG3   | 8                   | 0.12     | 0.01                | 0.12       |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD11 | 7                   | 1.14     | 0.92                | 0.63       |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD12 | 7                   | 1.14     | 0.92                | 0.63       |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD13 | 7                   | 1.14     | 0.92                | 0.63       |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD21 | 7                   | 1.14     | 0.92                | 0.63       |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD22 | 7                   | 1.14     | 0.92                | 0.63       |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD23 | 7                   | 1.14     | 0.92                | 0.63       |
| (2,1794) | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ3  | 7                   | 0.96     | 0.56                | 0.99       |
| (2,1794) | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ3  | 7                   | 0.96     | 0.56                | 0.99       |
| (2,1794) | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ3  | 7                   | 0.96     | 0.56                | 0.99       |
| (2,1794) | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ3  | 7                   | 0.96     | 0.56                | 0.99       |
| (2,1794) | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ3  | 7                   | 0.96     | 0.56                | 0.99       |
| (2,1794) | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ3  | 7                   | 0.96     | 0.56                | 0.99       |
| (2,1286) | 1:74:A:PHE:H     | 2:215:B:LYS:HG3  | 7                   | 0.94     | 0.56                | 1.17       |
| (2,14)   | 1:70:A:ILE:HD11  | 2:205:B:TRP:HZ3  | 7                   | 0.93     | 0.67                | 0.76       |
| (2,14)   | 1:70:A:ILE:HD12  | 2:205:B:TRP:HZ3  | 7                   | 0.93     | 0.67                | 0.76       |
| (2,14)   | 1:70:A:ILE:HD13  | 2:205:B:TRP:HZ3  | 7                   | 0.93     | 0.67                | 0.76       |
| (2,1206) | 1:73:A:ASP:HA    | 2:215:B:LYS:HG3  | 7                   | 0.81     | 0.5                 | 1.02       |
| (2,1267) | 2:205:B:TRP:HE3  | 2:220:B:ARG:HB3  | 7                   | 0.8      | 0.46                | 0.59       |
| (2,720)  | 1:74:A:PHE:H     | 2:215:B:LYS:HG2  | 7                   | 0.77     | 0.48                | 0.66       |
| (2,1486) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB3  | 7                   | 0.72     | 0.38                | 0.67       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,801)  | 1:74:A:PHE:H     | 2:214:B:LEU:HB2  | 7                   | 0.6      | 0.72                | 0.23       |
| (2,1930) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG2  | 7                   | 0.55     | 0.35                | 0.37       |
| (2,1930) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG2  | 7                   | 0.55     | 0.35                | 0.37       |
| (2,2140) | 2:208:B:GLN:HB2  | 2:217:B:ARG:HD2  | 7                   | 0.41     | 0.22                | 0.4        |
| (2,2140) | 2:208:B:GLN:HB2  | 2:217:B:ARG:HD3  | 7                   | 0.41     | 0.22                | 0.4        |
| (2,2140) | 2:208:B:GLN:HB3  | 2:217:B:ARG:HD2  | 7                   | 0.41     | 0.22                | 0.4        |
| (2,2140) | 2:208:B:GLN:HB3  | 2:217:B:ARG:HD3  | 7                   | 0.41     | 0.22                | 0.4        |
| (2,1438) | 2:203:B:LEU:HD11 | 2:204:B:THR:H    | 7                   | 0.37     | 0.1                 | 0.38       |
| (2,1438) | 2:203:B:LEU:HD12 | 2:204:B:THR:H    | 7                   | 0.37     | 0.1                 | 0.38       |
| (2,1438) | 2:203:B:LEU:HD13 | 2:204:B:THR:H    | 7                   | 0.37     | 0.1                 | 0.38       |
| (2,1202) | 2:215:B:LYS:HG2  | 2:216:B:ILE:H    | 7                   | 0.37     | 0.15                | 0.28       |
| (2,1187) | 2:217:B:ARG:HG2  | 2:218:B:LEU:H    | 7                   | 0.24     | 0.13                | 0.16       |
| (2,23)   | 1:70:A:ILE:HD11  | 2:205:B:TRP:HH2  | 6                   | 1.08     | 0.83                | 0.92       |
| (2,23)   | 1:70:A:ILE:HD12  | 2:205:B:TRP:HH2  | 6                   | 1.08     | 0.83                | 0.92       |
| (2,23)   | 1:70:A:ILE:HD13  | 2:205:B:TRP:HH2  | 6                   | 1.08     | 0.83                | 0.92       |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD11 | 6                   | 0.94     | 0.55                | 0.93       |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD12 | 6                   | 0.94     | 0.55                | 0.93       |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD13 | 6                   | 0.94     | 0.55                | 0.93       |
| (2,2109) | 2:206:B:ARG:HG2  | 2:220:B:ARG:HA   | 6                   | 0.87     | 0.41                | 1.04       |
| (2,2109) | 2:206:B:ARG:HG3  | 2:220:B:ARG:HA   | 6                   | 0.87     | 0.41                | 1.04       |
| (2,1174) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HB2  | 6                   | 0.85     | 0.89                | 0.49       |
| (2,101)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HH2  | 6                   | 0.8      | 0.51                | 0.65       |
| (2,101)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HH2  | 6                   | 0.8      | 0.51                | 0.65       |
| (2,101)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HH2  | 6                   | 0.8      | 0.51                | 0.65       |
| (2,1224) | 1:70:A:ILE:HD11  | 2:219:B:THR:HA   | 6                   | 0.78     | 0.31                | 0.78       |
| (2,1224) | 1:70:A:ILE:HD12  | 2:219:B:THR:HA   | 6                   | 0.78     | 0.31                | 0.78       |
| (2,1224) | 1:70:A:ILE:HD13  | 2:219:B:THR:HA   | 6                   | 0.78     | 0.31                | 0.78       |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG21 | 6                   | 0.77     | 0.26                | 0.77       |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG22 | 6                   | 0.77     | 0.26                | 0.77       |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG23 | 6                   | 0.77     | 0.26                | 0.77       |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD11 | 6                   | 0.69     | 0.33                | 0.79       |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD12 | 6                   | 0.69     | 0.33                | 0.79       |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD13 | 6                   | 0.69     | 0.33                | 0.79       |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD21 | 6                   | 0.69     | 0.33                | 0.79       |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD22 | 6                   | 0.69     | 0.33                | 0.79       |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD23 | 6                   | 0.69     | 0.33                | 0.79       |
| (2,1294) | 2:204:B:THR:HG21 | 2:205:B:TRP:HD1  | 6                   | 0.58     | 0.25                | 0.54       |
| (2,1294) | 2:204:B:THR:HG22 | 2:205:B:TRP:HD1  | 6                   | 0.58     | 0.25                | 0.54       |
| (2,1294) | 2:204:B:THR:HG23 | 2:205:B:TRP:HD1  | 6                   | 0.58     | 0.25                | 0.54       |
| (2,1367) | 1:73:A:ASP:HA    | 2:215:B:LYS:H    | 6                   | 0.55     | 0.32                | 0.55       |
| (2,1242) | 1:70:A:ILE:H     | 2:219:B:THR:HA   | 6                   | 0.55     | 0.17                | 0.54       |
| (2,1383) | 2:206:B:ARG:H    | 2:220:B:ARG:HA   | 6                   | 0.52     | 0.3                 | 0.46       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD11 | 6                   | 0.52     | 0.21                | 0.42       |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD12 | 6                   | 0.52     | 0.21                | 0.42       |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD13 | 6                   | 0.52     | 0.21                | 0.42       |
| (2,1233) | 2:204:B:THR:HG21 | 2:205:B:TRP:HB3  | 6                   | 0.42     | 0.2                 | 0.42       |
| (2,1233) | 2:204:B:THR:HG22 | 2:205:B:TRP:HB3  | 6                   | 0.42     | 0.2                 | 0.42       |
| (2,1233) | 2:204:B:THR:HG23 | 2:205:B:TRP:HB3  | 6                   | 0.42     | 0.2                 | 0.42       |
| (2,1392) | 2:209:B:ARG:HD3  | 2:210:B:SER:H    | 6                   | 0.4      | 0.32                | 0.29       |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD11 | 6                   | 0.34     | 0.21                | 0.29       |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD12 | 6                   | 0.34     | 0.21                | 0.29       |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD13 | 6                   | 0.34     | 0.21                | 0.29       |
| (2,2184) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HB3  | 6                   | 0.32     | 0.13                | 0.3        |
| (2,2184) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB3  | 6                   | 0.32     | 0.13                | 0.3        |
| (2,1736) | 1:48:A:LEU:HD11  | 2:205:B:TRP:H    | 6                   | 0.32     | 0.2                 | 0.29       |
| (2,1736) | 1:48:A:LEU:HD12  | 2:205:B:TRP:H    | 6                   | 0.32     | 0.2                 | 0.29       |
| (2,1736) | 1:48:A:LEU:HD13  | 2:205:B:TRP:H    | 6                   | 0.32     | 0.2                 | 0.29       |
| (2,1736) | 1:48:A:LEU:HD21  | 2:205:B:TRP:H    | 6                   | 0.32     | 0.2                 | 0.29       |
| (2,1736) | 1:48:A:LEU:HD22  | 2:205:B:TRP:H    | 6                   | 0.32     | 0.2                 | 0.29       |
| (2,1736) | 1:48:A:LEU:HD23  | 2:205:B:TRP:H    | 6                   | 0.32     | 0.2                 | 0.29       |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD11 | 6                   | 0.29     | 0.11                | 0.29       |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD12 | 6                   | 0.29     | 0.11                | 0.29       |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD13 | 6                   | 0.29     | 0.11                | 0.29       |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD21 | 6                   | 0.29     | 0.11                | 0.29       |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD22 | 6                   | 0.29     | 0.11                | 0.29       |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD23 | 6                   | 0.29     | 0.11                | 0.29       |
| (1,3)    | 1:34:A:ARG:O     | 1:38:A:LEU:N     | 6                   | 0.2      | 0.08                | 0.18       |
| (2,1500) | 1:20:A:GLU:HB2   | 1:21:A:GLU:H     | 6                   | 0.2      | 0.04                | 0.19       |
| (2,1500) | 1:20:A:GLU:HB3   | 1:21:A:GLU:H     | 6                   | 0.2      | 0.04                | 0.19       |
| (2,2050) | 1:90:A:LYS:HA    | 1:90:A:LYS:HD2   | 6                   | 0.2      | 0.05                | 0.18       |
| (2,2050) | 1:90:A:LYS:HA    | 1:90:A:LYS:HD3   | 6                   | 0.2      | 0.05                | 0.18       |
| (2,1503) | 1:22:A:GLU:HB2   | 1:23:A:GLU:H     | 6                   | 0.17     | 0.05                | 0.18       |
| (2,1503) | 1:22:A:GLU:HB3   | 1:23:A:GLU:H     | 6                   | 0.17     | 0.05                | 0.18       |
| (2,1965) | 1:77:A:LEU:HD11  | 1:78:A:LYS:HB2   | 6                   | 0.13     | 0.03                | 0.12       |
| (2,1965) | 1:77:A:LEU:HD12  | 1:78:A:LYS:HB2   | 6                   | 0.13     | 0.03                | 0.12       |
| (2,1965) | 1:77:A:LEU:HD13  | 1:78:A:LYS:HB2   | 6                   | 0.13     | 0.03                | 0.12       |
| (2,1965) | 1:77:A:LEU:HD21  | 1:78:A:LYS:HB2   | 6                   | 0.13     | 0.03                | 0.12       |
| (2,1965) | 1:77:A:LEU:HD22  | 1:78:A:LYS:HB2   | 6                   | 0.13     | 0.03                | 0.12       |
| (2,1965) | 1:77:A:LEU:HD23  | 1:78:A:LYS:HB2   | 6                   | 0.13     | 0.03                | 0.12       |
| (2,76)   | 1:75:A:GLU:HG3   | 2:214:B:LEU:HB2  | 5                   | 1.59     | 0.63                | 1.26       |
| (2,2200) | 2:214:B:LEU:HD11 | 2:215:B:LYS:HG3  | 5                   | 1.23     | 0.61                | 1.36       |
| (2,2200) | 2:214:B:LEU:HD12 | 2:215:B:LYS:HG3  | 5                   | 1.23     | 0.61                | 1.36       |
| (2,2200) | 2:214:B:LEU:HD13 | 2:215:B:LYS:HG3  | 5                   | 1.23     | 0.61                | 1.36       |
| (2,2200) | 2:214:B:LEU:HD21 | 2:215:B:LYS:HG3  | 5                   | 1.23     | 0.61                | 1.36       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,2200) | 2:214:B:LEU:HD22 | 2:215:B:LYS:HG3  | 5                   | 1.23     | 0.61                | 1.36       |
| (2,2200) | 2:214:B:LEU:HD23 | 2:215:B:LYS:HG3  | 5                   | 1.23     | 0.61                | 1.36       |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD11 | 5                   | 1.21     | 0.65                | 1.25       |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD12 | 5                   | 1.21     | 0.65                | 1.25       |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD13 | 5                   | 1.21     | 0.65                | 1.25       |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 5                   | 1.21     | 0.65                | 1.25       |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 5                   | 1.21     | 0.65                | 1.25       |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 5                   | 1.21     | 0.65                | 1.25       |
| (2,615)  | 1:75:A:GLU:HG2   | 2:214:B:LEU:HB2  | 5                   | 1.16     | 0.72                | 0.74       |
| (2,1333) | 1:34:A:ARG:HG2   | 2:213:B:PRO:HG3  | 5                   | 1.03     | 0.42                | 1.16       |
| (2,613)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ2  | 5                   | 0.98     | 0.41                | 1.15       |
| (2,613)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ2  | 5                   | 0.98     | 0.41                | 1.15       |
| (2,613)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ2  | 5                   | 0.98     | 0.41                | 1.15       |
| (2,160)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ3  | 5                   | 0.9      | 0.36                | 0.7        |
| (2,160)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ3  | 5                   | 0.9      | 0.36                | 0.7        |
| (2,160)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ3  | 5                   | 0.9      | 0.36                | 0.7        |
| (2,1489) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE3  | 5                   | 0.84     | 0.39                | 0.91       |
| (2,1910) | 1:69:A:GLU:HG2   | 2:219:B:THR:HG21 | 5                   | 0.68     | 0.35                | 0.79       |
| (2,1910) | 1:69:A:GLU:HG2   | 2:219:B:THR:HG22 | 5                   | 0.68     | 0.35                | 0.79       |
| (2,1910) | 1:69:A:GLU:HG2   | 2:219:B:THR:HG23 | 5                   | 0.68     | 0.35                | 0.79       |
| (2,1910) | 1:69:A:GLU:HG3   | 2:219:B:THR:HG21 | 5                   | 0.68     | 0.35                | 0.79       |
| (2,1910) | 1:69:A:GLU:HG3   | 2:219:B:THR:HG22 | 5                   | 0.68     | 0.35                | 0.79       |
| (2,1910) | 1:69:A:GLU:HG3   | 2:219:B:THR:HG23 | 5                   | 0.68     | 0.35                | 0.79       |
| (2,1398) | 1:68:A:ASP:HB2   | 2:220:B:ARG:H    | 5                   | 0.66     | 0.42                | 0.37       |
| (2,2172) | 2:210:B:SER:HB2  | 2:215:B:LYS:HD2  | 5                   | 0.64     | 0.29                | 0.51       |
| (2,2172) | 2:210:B:SER:HB3  | 2:215:B:LYS:HD2  | 5                   | 0.64     | 0.29                | 0.51       |
| (2,1225) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HA   | 5                   | 0.64     | 0.39                | 0.64       |
| (2,176)  | 1:73:A:ASP:HA    | 2:215:B:LYS:HD3  | 5                   | 0.53     | 0.17                | 0.41       |
| (2,1455) | 1:74:A:PHE:H     | 2:214:B:LEU:H    | 5                   | 0.52     | 0.25                | 0.53       |
| (2,1909) | 1:69:A:GLU:HG2   | 2:219:B:THR:HB   | 5                   | 0.48     | 0.19                | 0.4        |
| (2,1909) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 5                   | 0.48     | 0.19                | 0.4        |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD11 | 5                   | 0.48     | 0.32                | 0.4        |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD12 | 5                   | 0.48     | 0.32                | 0.4        |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD13 | 5                   | 0.48     | 0.32                | 0.4        |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD21 | 5                   | 0.48     | 0.32                | 0.4        |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD22 | 5                   | 0.48     | 0.32                | 0.4        |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD23 | 5                   | 0.48     | 0.32                | 0.4        |
| (2,2165) | 2:209:B:ARG:HD2  | 2:210:B:SER:H    | 5                   | 0.46     | 0.33                | 0.3        |
| (2,2165) | 2:209:B:ARG:HD3  | 2:210:B:SER:H    | 5                   | 0.46     | 0.33                | 0.3        |
| (2,1403) | 2:221:B:GLU:HB3  | 2:222:B:ALA:H    | 5                   | 0.37     | 0.14                | 0.44       |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD11 | 5                   | 0.37     | 0.13                | 0.38       |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD12 | 5                   | 0.37     | 0.13                | 0.38       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD13 | 5                   | 0.37     | 0.13                | 0.38       |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD21 | 5                   | 0.37     | 0.13                | 0.38       |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD22 | 5                   | 0.37     | 0.13                | 0.38       |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD23 | 5                   | 0.37     | 0.13                | 0.38       |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD11 | 5                   | 0.37     | 0.13                | 0.38       |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD12 | 5                   | 0.37     | 0.13                | 0.38       |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD13 | 5                   | 0.37     | 0.13                | 0.38       |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD21 | 5                   | 0.37     | 0.13                | 0.38       |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD22 | 5                   | 0.37     | 0.13                | 0.38       |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD23 | 5                   | 0.37     | 0.13                | 0.38       |
| (2,2122) | 2:207:B:VAL:HG11 | 2:217:B:ARG:H    | 5                   | 0.33     | 0.13                | 0.37       |
| (2,2122) | 2:207:B:VAL:HG12 | 2:217:B:ARG:H    | 5                   | 0.33     | 0.13                | 0.37       |
| (2,2122) | 2:207:B:VAL:HG13 | 2:217:B:ARG:H    | 5                   | 0.33     | 0.13                | 0.37       |
| (2,2122) | 2:207:B:VAL:HG21 | 2:217:B:ARG:H    | 5                   | 0.33     | 0.13                | 0.37       |
| (2,2122) | 2:207:B:VAL:HG22 | 2:217:B:ARG:H    | 5                   | 0.33     | 0.13                | 0.37       |
| (2,2122) | 2:207:B:VAL:HG23 | 2:217:B:ARG:H    | 5                   | 0.33     | 0.13                | 0.37       |
| (2,1353) | 1:74:A:PHE:HD1   | 2:215:B:LYS:H    | 5                   | 0.32     | 0.17                | 0.27       |
| (2,1353) | 1:74:A:PHE:HD2   | 2:215:B:LYS:H    | 5                   | 0.32     | 0.17                | 0.27       |
| (2,1415) | 1:70:A:ILE:HB    | 2:218:B:LEU:H    | 5                   | 0.26     | 0.09                | 0.3        |
| (2,1738) | 1:48:A:LEU:HD11  | 2:206:B:ARG:H    | 5                   | 0.26     | 0.04                | 0.25       |
| (2,1738) | 1:48:A:LEU:HD12  | 2:206:B:ARG:H    | 5                   | 0.26     | 0.04                | 0.25       |
| (2,1738) | 1:48:A:LEU:HD13  | 2:206:B:ARG:H    | 5                   | 0.26     | 0.04                | 0.25       |
| (2,1738) | 1:48:A:LEU:HD21  | 2:206:B:ARG:H    | 5                   | 0.26     | 0.04                | 0.25       |
| (2,1738) | 1:48:A:LEU:HD22  | 2:206:B:ARG:H    | 5                   | 0.26     | 0.04                | 0.25       |
| (2,1738) | 1:48:A:LEU:HD23  | 2:206:B:ARG:H    | 5                   | 0.26     | 0.04                | 0.25       |
| (2,799)  | 1:22:A:GLU:HB2   | 1:23:A:GLU:H     | 5                   | 0.21     | 0.06                | 0.18       |
| (2,152)  | 1:34:A:ARG:HA    | 2:214:B:LEU:HG   | 5                   | 0.2      | 0.04                | 0.19       |
| (2,1102) | 1:75:A:GLU:H     | 2:215:B:LYS:HA   | 5                   | 0.18     | 0.07                | 0.19       |
| (2,1805) | 1:54:A:ILE:HG21  | 1:84:A:GLU:HB2   | 5                   | 0.16     | 0.04                | 0.17       |
| (2,1805) | 1:54:A:ILE:HG21  | 1:84:A:GLU:HB3   | 5                   | 0.16     | 0.04                | 0.17       |
| (2,1805) | 1:54:A:ILE:HG22  | 1:84:A:GLU:HB2   | 5                   | 0.16     | 0.04                | 0.17       |
| (2,1805) | 1:54:A:ILE:HG22  | 1:84:A:GLU:HB3   | 5                   | 0.16     | 0.04                | 0.17       |
| (2,1805) | 1:54:A:ILE:HG23  | 1:84:A:GLU:HB2   | 5                   | 0.16     | 0.04                | 0.17       |
| (2,1805) | 1:54:A:ILE:HG23  | 1:84:A:GLU:HB3   | 5                   | 0.16     | 0.04                | 0.17       |
| (2,803)  | 1:75:A:GLU:H     | 2:214:B:LEU:HB2  | 4                   | 0.97     | 0.76                | 0.64       |
| (2,752)  | 1:75:A:GLU:H     | 2:214:B:LEU:HG   | 4                   | 0.86     | 0.49                | 0.86       |
| (2,1488) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HD3  | 4                   | 0.84     | 0.17                | 0.92       |
| (2,1929) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HA   | 4                   | 0.64     | 0.23                | 0.64       |
| (2,1929) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HA   | 4                   | 0.64     | 0.23                | 0.64       |
| (2,2187) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE2  | 4                   | 0.62     | 0.37                | 0.51       |
| (2,2187) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE3  | 4                   | 0.62     | 0.37                | 0.51       |
| (2,636)  | 1:69:A:GLU:HA    | 2:219:B:THR:HG21 | 4                   | 0.6      | 0.26                | 0.65       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (2,636)  | 1:69:A:GLU:HA   | 2:219:B:THR:HG22 | 4                   | 0.6      | 0.26                | 0.65       |
| (2,636)  | 1:69:A:GLU:HA   | 2:219:B:THR:HG23 | 4                   | 0.6      | 0.26                | 0.65       |
| (2,1355) | 1:74:A:PHE:HD1  | 2:214:B:LEU:H    | 4                   | 0.58     | 0.3                 | 0.5        |
| (2,1355) | 1:74:A:PHE:HD2  | 2:214:B:LEU:H    | 4                   | 0.58     | 0.3                 | 0.5        |
| (2,2084) | 2:205:B:TRP:H   | 2:220:B:ARG:HG2  | 4                   | 0.57     | 0.41                | 0.48       |
| (2,2084) | 2:205:B:TRP:H   | 2:220:B:ARG:HG3  | 4                   | 0.57     | 0.41                | 0.48       |
| (2,1214) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD11 | 4                   | 0.56     | 0.41                | 0.56       |
| (2,1214) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD12 | 4                   | 0.56     | 0.41                | 0.56       |
| (2,1214) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD13 | 4                   | 0.56     | 0.41                | 0.56       |
| (2,177)  | 1:73:A:ASP:HA   | 2:216:B:ILE:HG21 | 4                   | 0.53     | 0.22                | 0.53       |
| (2,177)  | 1:73:A:ASP:HA   | 2:216:B:ILE:HG22 | 4                   | 0.53     | 0.22                | 0.53       |
| (2,177)  | 1:73:A:ASP:HA   | 2:216:B:ILE:HG23 | 4                   | 0.53     | 0.22                | 0.53       |
| (2,965)  | 1:74:A:PHE:H    | 2:214:B:LEU:HA   | 4                   | 0.48     | 0.24                | 0.45       |
| (2,1257) | 1:73:A:ASP:HA   | 2:215:B:LYS:HB2  | 4                   | 0.46     | 0.23                | 0.46       |
| (2,1152) | 1:74:A:PHE:HD1  | 2:214:B:LEU:HA   | 4                   | 0.45     | 0.14                | 0.44       |
| (2,1152) | 1:74:A:PHE:HD2  | 2:214:B:LEU:HA   | 4                   | 0.45     | 0.14                | 0.44       |
| (2,1104) | 1:73:A:ASP:H    | 2:215:B:LYS:HA   | 4                   | 0.44     | 0.19                | 0.36       |
| (2,1358) | 2:205:B:TRP:HD1 | 2:206:B:ARG:H    | 4                   | 0.41     | 0.25                | 0.32       |
| (2,2141) | 2:208:B:GLN:HB2 | 2:219:B:THR:H    | 4                   | 0.39     | 0.27                | 0.26       |
| (2,2141) | 2:208:B:GLN:HB3 | 2:219:B:THR:H    | 4                   | 0.39     | 0.27                | 0.26       |
| (2,2216) | 2:217:B:ARG:HD2 | 2:219:B:THR:HB   | 4                   | 0.34     | 0.09                | 0.34       |
| (2,2216) | 2:217:B:ARG:HD3 | 2:219:B:THR:HB   | 4                   | 0.34     | 0.09                | 0.34       |
| (2,30)   | 1:30:A:TYR:HE1  | 2:214:B:LEU:HG   | 4                   | 0.32     | 0.18                | 0.28       |
| (2,30)   | 1:30:A:TYR:HE2  | 2:214:B:LEU:HG   | 4                   | 0.32     | 0.18                | 0.28       |
| (2,1471) | 1:74:A:PHE:H    | 2:215:B:LYS:H    | 4                   | 0.31     | 0.14                | 0.34       |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD11 | 4                   | 0.26     | 0.13                | 0.24       |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD12 | 4                   | 0.26     | 0.13                | 0.24       |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD13 | 4                   | 0.26     | 0.13                | 0.24       |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD21 | 4                   | 0.26     | 0.13                | 0.24       |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD22 | 4                   | 0.26     | 0.13                | 0.24       |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD23 | 4                   | 0.26     | 0.13                | 0.24       |
| (2,2132) | 2:208:B:GLN:H   | 2:218:B:LEU:HD11 | 4                   | 0.24     | 0.06                | 0.24       |
| (2,2132) | 2:208:B:GLN:H   | 2:218:B:LEU:HD12 | 4                   | 0.24     | 0.06                | 0.24       |
| (2,2132) | 2:208:B:GLN:H   | 2:218:B:LEU:HD13 | 4                   | 0.24     | 0.06                | 0.24       |
| (2,2132) | 2:208:B:GLN:H   | 2:218:B:LEU:HD21 | 4                   | 0.24     | 0.06                | 0.24       |
| (2,2132) | 2:208:B:GLN:H   | 2:218:B:LEU:HD22 | 4                   | 0.24     | 0.06                | 0.24       |
| (2,2132) | 2:208:B:GLN:H   | 2:218:B:LEU:HD23 | 4                   | 0.24     | 0.06                | 0.24       |
| (2,1406) | 2:214:B:LEU:HB2 | 2:215:B:LYS:H    | 4                   | 0.24     | 0.19                | 0.14       |
| (2,1464) | 2:205:B:TRP:HD1 | 2:221:B:GLU:H    | 4                   | 0.23     | 0.01                | 0.23       |
| (2,1546) | 1:28:A:MET:HE1  | 1:33:A:LYS:HD2   | 4                   | 0.22     | 0.07                | 0.22       |
| (2,1546) | 1:28:A:MET:HE1  | 1:33:A:LYS:HD3   | 4                   | 0.22     | 0.07                | 0.22       |
| (2,1546) | 1:28:A:MET:HE2  | 1:33:A:LYS:HD2   | 4                   | 0.22     | 0.07                | 0.22       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1546) | 1:28:A:MET:HE2   | 1:33:A:LYS:HD3   | 4                   | 0.22     | 0.07                | 0.22       |
| (2,1546) | 1:28:A:MET:HE3   | 1:33:A:LYS:HD2   | 4                   | 0.22     | 0.07                | 0.22       |
| (2,1546) | 1:28:A:MET:HE3   | 1:33:A:LYS:HD3   | 4                   | 0.22     | 0.07                | 0.22       |
| (2,432)  | 1:53:A:HIS:HA    | 1:56:A:GLN:HB3   | 4                   | 0.18     | 0.05                | 0.18       |
| (2,1865) | 1:62:A:LEU:HB2   | 1:65:A:SER:HB2   | 4                   | 0.18     | 0.02                | 0.18       |
| (2,1865) | 1:62:A:LEU:HB2   | 1:65:A:SER:HB3   | 4                   | 0.18     | 0.02                | 0.18       |
| (2,1865) | 1:62:A:LEU:HB3   | 1:65:A:SER:HB2   | 4                   | 0.18     | 0.02                | 0.18       |
| (2,1865) | 1:62:A:LEU:HB3   | 1:65:A:SER:HB3   | 4                   | 0.18     | 0.02                | 0.18       |
| (2,1208) | 2:215:B:LYS:HA   | 2:215:B:LYS:HD2  | 4                   | 0.18     | 0.02                | 0.18       |
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD11  | 4                   | 0.15     | 0.04                | 0.15       |
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD12  | 4                   | 0.15     | 0.04                | 0.15       |
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD13  | 4                   | 0.15     | 0.04                | 0.15       |
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD21  | 4                   | 0.15     | 0.04                | 0.15       |
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD22  | 4                   | 0.15     | 0.04                | 0.15       |
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD23  | 4                   | 0.15     | 0.04                | 0.15       |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD11  | 4                   | 0.15     | 0.04                | 0.15       |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD12  | 4                   | 0.15     | 0.04                | 0.15       |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD13  | 4                   | 0.15     | 0.04                | 0.15       |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD21  | 4                   | 0.15     | 0.04                | 0.15       |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD22  | 4                   | 0.15     | 0.04                | 0.15       |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD23  | 4                   | 0.15     | 0.04                | 0.15       |
| (2,1321) | 2:221:B:GLU:HB2  | 2:222:B:ALA:H    | 4                   | 0.15     | 0.01                | 0.14       |
| (2,1175) | 2:210:B:SER:HB3  | 2:215:B:LYS:HB3  | 3                   | 1.3      | 0.8                 | 0.83       |
| (2,2154) | 2:208:B:GLN:HE22 | 2:217:B:ARG:HD2  | 3                   | 1.19     | 0.54                | 1.57       |
| (2,2154) | 2:208:B:GLN:HE22 | 2:217:B:ARG:HD3  | 3                   | 1.19     | 0.54                | 1.57       |
| (2,1209) | 1:73:A:ASP:HA    | 2:215:B:LYS:HD2  | 3                   | 1.16     | 0.1                 | 1.18       |
| (2,1484) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HG3  | 3                   | 1.08     | 0.25                | 1.2        |
| (2,2170) | 2:210:B:SER:HB2  | 2:215:B:LYS:H    | 3                   | 1.04     | 0.17                | 0.93       |
| (2,2170) | 2:210:B:SER:HB3  | 2:215:B:LYS:H    | 3                   | 1.04     | 0.17                | 0.93       |
| (2,2153) | 2:208:B:GLN:HG2  | 2:219:B:THR:HG21 | 3                   | 1.02     | 0.42                | 1.1        |
| (2,2153) | 2:208:B:GLN:HG2  | 2:219:B:THR:HG22 | 3                   | 1.02     | 0.42                | 1.1        |
| (2,2153) | 2:208:B:GLN:HG2  | 2:219:B:THR:HG23 | 3                   | 1.02     | 0.42                | 1.1        |
| (2,2153) | 2:208:B:GLN:HG3  | 2:219:B:THR:HG21 | 3                   | 1.02     | 0.42                | 1.1        |
| (2,2153) | 2:208:B:GLN:HG3  | 2:219:B:THR:HG22 | 3                   | 1.02     | 0.42                | 1.1        |
| (2,2153) | 2:208:B:GLN:HG3  | 2:219:B:THR:HG23 | 3                   | 1.02     | 0.42                | 1.1        |
| (2,2110) | 2:206:B:ARG:HG2  | 2:221:B:GLU:H    | 3                   | 0.88     | 0.35                | 0.71       |
| (2,2110) | 2:206:B:ARG:HG3  | 2:221:B:GLU:H    | 3                   | 0.88     | 0.35                | 0.71       |
| (2,1178) | 2:210:B:SER:HB3  | 2:215:B:LYS:HB2  | 3                   | 0.86     | 0.21                | 0.9        |
| (2,1908) | 1:69:A:GLU:HG2   | 2:217:B:ARG:HD2  | 3                   | 0.84     | 0.18                | 0.74       |
| (2,1908) | 1:69:A:GLU:HG2   | 2:217:B:ARG:HD3  | 3                   | 0.84     | 0.18                | 0.74       |
| (2,1908) | 1:69:A:GLU:HG3   | 2:217:B:ARG:HD2  | 3                   | 0.84     | 0.18                | 0.74       |
| (2,1908) | 1:69:A:GLU:HG3   | 2:217:B:ARG:HD3  | 3                   | 0.84     | 0.18                | 0.74       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (2,1176) | 2:210:B:SER:HB2 | 2:215:B:LYS:HB3  | 3                   | 0.83     | 0.49                | 1.15       |
| (2,1932) | 1:73:A:ASP:HB2  | 2:215:B:LYS:HD3  | 3                   | 0.7      | 0.11                | 0.68       |
| (2,1932) | 1:73:A:ASP:HB3  | 2:215:B:LYS:HD3  | 3                   | 0.7      | 0.11                | 0.68       |
| (2,1243) | 2:205:B:TRP:HA  | 2:220:B:ARG:HG2  | 3                   | 0.7      | 0.04                | 0.71       |
| (2,1418) | 2:214:B:LEU:H   | 2:215:B:LYS:HB2  | 3                   | 0.68     | 0.43                | 0.67       |
| (2,616)  | 1:75:A:GLU:HA   | 2:214:B:LEU:HG   | 3                   | 0.63     | 0.11                | 0.61       |
| (2,1227) | 1:73:A:ASP:HB2  | 2:215:B:LYS:HA   | 3                   | 0.63     | 0.18                | 0.63       |
| (2,1204) | 1:73:A:ASP:HA   | 2:215:B:LYS:HG2  | 3                   | 0.61     | 0.36                | 0.46       |
| (2,95)   | 1:74:A:PHE:HB2  | 2:214:B:LEU:HA   | 3                   | 0.57     | 0.03                | 0.57       |
| (1,1)    | 1:33:A:LYS:O    | 1:37:A:SER:N     | 3                   | 0.53     | 0.18                | 0.64       |
| (2,1391) | 2:209:B:ARG:HD2 | 2:210:B:SER:H    | 3                   | 0.53     | 0.42                | 0.32       |
| (2,2094) | 2:205:B:TRP:HE3 | 2:220:B:ARG:HB2  | 3                   | 0.53     | 0.13                | 0.61       |
| (2,2094) | 2:205:B:TRP:HE3 | 2:220:B:ARG:HB3  | 3                   | 0.53     | 0.13                | 0.61       |
| (2,2118) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD11 | 3                   | 0.52     | 0.13                | 0.46       |
| (2,2118) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD12 | 3                   | 0.52     | 0.13                | 0.46       |
| (2,2118) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD13 | 3                   | 0.52     | 0.13                | 0.46       |
| (2,2118) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD21 | 3                   | 0.52     | 0.13                | 0.46       |
| (2,2118) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD22 | 3                   | 0.52     | 0.13                | 0.46       |
| (2,2118) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD23 | 3                   | 0.52     | 0.13                | 0.46       |
| (1,2)    | 1:33:A:LYS:O    | 1:37:A:SER:H     | 3                   | 0.51     | 0.2                 | 0.63       |
| (2,1253) | 2:214:B:LEU:HG  | 2:215:B:LYS:H    | 3                   | 0.44     | 0.23                | 0.5        |
| (2,1397) | 2:205:B:TRP:HB2 | 2:220:B:ARG:H    | 3                   | 0.44     | 0.23                | 0.54       |
| (2,1795) | 1:52:A:VAL:HG11 | 2:205:B:TRP:HZ2  | 3                   | 0.41     | 0.13                | 0.4        |
| (2,1795) | 1:52:A:VAL:HG12 | 2:205:B:TRP:HZ2  | 3                   | 0.41     | 0.13                | 0.4        |
| (2,1795) | 1:52:A:VAL:HG13 | 2:205:B:TRP:HZ2  | 3                   | 0.41     | 0.13                | 0.4        |
| (2,1795) | 1:52:A:VAL:HG21 | 2:205:B:TRP:HZ2  | 3                   | 0.41     | 0.13                | 0.4        |
| (2,1795) | 1:52:A:VAL:HG22 | 2:205:B:TRP:HZ2  | 3                   | 0.41     | 0.13                | 0.4        |
| (2,1795) | 1:52:A:VAL:HG23 | 2:205:B:TRP:HZ2  | 3                   | 0.41     | 0.13                | 0.4        |
| (2,619)  | 1:72:A:ILE:HB   | 2:216:B:ILE:HB   | 3                   | 0.4      | 0.18                | 0.52       |
| (2,1605) | 1:34:A:ARG:HD2  | 2:213:B:PRO:HB2  | 3                   | 0.39     | 0.21                | 0.47       |
| (2,1605) | 1:34:A:ARG:HD2  | 2:213:B:PRO:HB3  | 3                   | 0.39     | 0.21                | 0.47       |
| (2,1605) | 1:34:A:ARG:HD3  | 2:213:B:PRO:HB2  | 3                   | 0.39     | 0.21                | 0.47       |
| (2,1605) | 1:34:A:ARG:HD3  | 2:213:B:PRO:HB3  | 3                   | 0.39     | 0.21                | 0.47       |
| (2,1331) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD21 | 3                   | 0.37     | 0.24                | 0.28       |
| (2,1331) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD22 | 3                   | 0.37     | 0.24                | 0.28       |
| (2,1331) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD23 | 3                   | 0.37     | 0.24                | 0.28       |
| (2,2169) | 2:210:B:SER:HB2 | 2:212:B:ASN:H    | 3                   | 0.34     | 0.17                | 0.4        |
| (2,2169) | 2:210:B:SER:HB3 | 2:212:B:ASN:H    | 3                   | 0.34     | 0.17                | 0.4        |
| (2,2113) | 2:206:B:ARG:HD2 | 2:221:B:GLU:HG2  | 3                   | 0.33     | 0.18                | 0.28       |
| (2,2113) | 2:206:B:ARG:HD2 | 2:221:B:GLU:HG3  | 3                   | 0.33     | 0.18                | 0.28       |
| (2,2113) | 2:206:B:ARG:HD3 | 2:221:B:GLU:HG2  | 3                   | 0.33     | 0.18                | 0.28       |
| (2,2113) | 2:206:B:ARG:HD3 | 2:221:B:GLU:HG3  | 3                   | 0.33     | 0.18                | 0.28       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1288) | 1:52:A:VAL:HG21  | 2:218:B:LEU:HG   | 3                   | 0.31     | 0.14                | 0.22       |
| (2,1288) | 1:52:A:VAL:HG22  | 2:218:B:LEU:HG   | 3                   | 0.31     | 0.14                | 0.22       |
| (2,1288) | 1:52:A:VAL:HG23  | 2:218:B:LEU:HG   | 3                   | 0.31     | 0.14                | 0.22       |
| (2,1903) | 1:68:A:ASP:HB3   | 2:220:B:ARG:HG2  | 3                   | 0.3      | 0.13                | 0.38       |
| (2,1903) | 1:68:A:ASP:HB3   | 2:220:B:ARG:HG3  | 3                   | 0.3      | 0.13                | 0.38       |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD11 | 3                   | 0.26     | 0.04                | 0.26       |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD12 | 3                   | 0.26     | 0.04                | 0.26       |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD13 | 3                   | 0.26     | 0.04                | 0.26       |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD21 | 3                   | 0.26     | 0.04                | 0.26       |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD22 | 3                   | 0.26     | 0.04                | 0.26       |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD23 | 3                   | 0.26     | 0.04                | 0.26       |
| (2,1740) | 1:48:A:LEU:HD11  | 2:206:B:ARG:HB2  | 3                   | 0.24     | 0.14                | 0.19       |
| (2,1740) | 1:48:A:LEU:HD11  | 2:206:B:ARG:HB3  | 3                   | 0.24     | 0.14                | 0.19       |
| (2,1740) | 1:48:A:LEU:HD12  | 2:206:B:ARG:HB2  | 3                   | 0.24     | 0.14                | 0.19       |
| (2,1740) | 1:48:A:LEU:HD12  | 2:206:B:ARG:HB3  | 3                   | 0.24     | 0.14                | 0.19       |
| (2,1740) | 1:48:A:LEU:HD13  | 2:206:B:ARG:HB2  | 3                   | 0.24     | 0.14                | 0.19       |
| (2,1740) | 1:48:A:LEU:HD13  | 2:206:B:ARG:HB3  | 3                   | 0.24     | 0.14                | 0.19       |
| (2,1740) | 1:48:A:LEU:HD21  | 2:206:B:ARG:HB2  | 3                   | 0.24     | 0.14                | 0.19       |
| (2,1740) | 1:48:A:LEU:HD21  | 2:206:B:ARG:HB3  | 3                   | 0.24     | 0.14                | 0.19       |
| (2,1740) | 1:48:A:LEU:HD22  | 2:206:B:ARG:HB2  | 3                   | 0.24     | 0.14                | 0.19       |
| (2,1740) | 1:48:A:LEU:HD22  | 2:206:B:ARG:HB3  | 3                   | 0.24     | 0.14                | 0.19       |
| (2,1740) | 1:48:A:LEU:HD23  | 2:206:B:ARG:HB2  | 3                   | 0.24     | 0.14                | 0.19       |
| (2,1740) | 1:48:A:LEU:HD23  | 2:206:B:ARG:HB3  | 3                   | 0.24     | 0.14                | 0.19       |
| (2,1545) | 1:28:A:MET:HE1   | 1:33:A:LYS:HG2   | 3                   | 0.23     | 0.07                | 0.25       |
| (2,1545) | 1:28:A:MET:HE1   | 1:33:A:LYS:HG3   | 3                   | 0.23     | 0.07                | 0.25       |
| (2,1545) | 1:28:A:MET:HE2   | 1:33:A:LYS:HG2   | 3                   | 0.23     | 0.07                | 0.25       |
| (2,1545) | 1:28:A:MET:HE2   | 1:33:A:LYS:HG3   | 3                   | 0.23     | 0.07                | 0.25       |
| (2,1545) | 1:28:A:MET:HE3   | 1:33:A:LYS:HG2   | 3                   | 0.23     | 0.07                | 0.25       |
| (2,1545) | 1:28:A:MET:HE3   | 1:33:A:LYS:HG3   | 3                   | 0.23     | 0.07                | 0.25       |
| (2,2123) | 2:207:B:VAL:HG11 | 2:217:B:ARG:HA   | 3                   | 0.21     | 0.1                 | 0.17       |
| (2,2123) | 2:207:B:VAL:HG12 | 2:217:B:ARG:HA   | 3                   | 0.21     | 0.1                 | 0.17       |
| (2,2123) | 2:207:B:VAL:HG13 | 2:217:B:ARG:HA   | 3                   | 0.21     | 0.1                 | 0.17       |
| (2,2123) | 2:207:B:VAL:HG21 | 2:217:B:ARG:HA   | 3                   | 0.21     | 0.1                 | 0.17       |
| (2,2123) | 2:207:B:VAL:HG22 | 2:217:B:ARG:HA   | 3                   | 0.21     | 0.1                 | 0.17       |
| (2,2123) | 2:207:B:VAL:HG23 | 2:217:B:ARG:HA   | 3                   | 0.21     | 0.1                 | 0.17       |
| (2,633)  | 1:71:A:GLU:HG3   | 2:217:B:ARG:HG2  | 3                   | 0.21     | 0.05                | 0.21       |
| (2,2171) | 2:210:B:SER:HB2  | 2:215:B:LYS:HB2  | 3                   | 0.19     | 0.04                | 0.21       |
| (2,2171) | 2:210:B:SER:HB3  | 2:215:B:LYS:HB2  | 3                   | 0.19     | 0.04                | 0.21       |
| (2,1357) | 2:205:B:TRP:H    | 2:205:B:TRP:HD1  | 3                   | 0.17     | 0.09                | 0.12       |
| (2,1451) | 1:71:A:GLU:HG3   | 2:218:B:LEU:H    | 3                   | 0.17     | 0.05                | 0.17       |
| (2,310)  | 1:37:A:SER:HA    | 1:40:A:ILE:HD11  | 3                   | 0.13     | 0.01                | 0.13       |
| (2,310)  | 1:37:A:SER:HA    | 1:40:A:ILE:HD12  | 3                   | 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,310)  | 1:37:A:SER:HA    | 1:40:A:ILE:HD13  | 3                   | 0.13     | 0.01                | 0.13       |
| (2,1534) | 1:28:A:MET:H     | 1:82:A:LEU:HD11  | 3                   | 0.11     | 0.02                | 0.1        |
| (2,1534) | 1:28:A:MET:H     | 1:82:A:LEU:HD12  | 3                   | 0.11     | 0.02                | 0.1        |
| (2,1534) | 1:28:A:MET:H     | 1:82:A:LEU:HD13  | 3                   | 0.11     | 0.02                | 0.1        |
| (2,1534) | 1:28:A:MET:H     | 1:82:A:LEU:HD21  | 3                   | 0.11     | 0.02                | 0.1        |
| (2,1534) | 1:28:A:MET:H     | 1:82:A:LEU:HD22  | 3                   | 0.11     | 0.02                | 0.1        |
| (2,1534) | 1:28:A:MET:H     | 1:82:A:LEU:HD23  | 3                   | 0.11     | 0.02                | 0.1        |
| (2,1527) | 1:26:A:LEU:HD11  | 1:27:A:PRO:HD2   | 3                   | 0.11     | 0.01                | 0.11       |
| (2,1527) | 1:26:A:LEU:HD12  | 1:27:A:PRO:HD2   | 3                   | 0.11     | 0.01                | 0.11       |
| (2,1527) | 1:26:A:LEU:HD13  | 1:27:A:PRO:HD2   | 3                   | 0.11     | 0.01                | 0.11       |
| (2,1527) | 1:26:A:LEU:HD21  | 1:27:A:PRO:HD2   | 3                   | 0.11     | 0.01                | 0.11       |
| (2,1527) | 1:26:A:LEU:HD22  | 1:27:A:PRO:HD2   | 3                   | 0.11     | 0.01                | 0.11       |
| (2,1527) | 1:26:A:LEU:HD23  | 1:27:A:PRO:HD2   | 3                   | 0.11     | 0.01                | 0.11       |
| (2,1426) | 2:214:B:LEU:H    | 2:215:B:LYS:HG3  | 2                   | 1.14     | 0.39                | 1.14       |
| (2,2111) | 2:206:B:ARG:HG2  | 2:221:B:GLU:HG2  | 2                   | 0.98     | 0.26                | 0.98       |
| (2,2111) | 2:206:B:ARG:HG2  | 2:221:B:GLU:HG3  | 2                   | 0.98     | 0.26                | 0.98       |
| (2,2111) | 2:206:B:ARG:HG3  | 2:221:B:GLU:HG2  | 2                   | 0.98     | 0.26                | 0.98       |
| (2,2111) | 2:206:B:ARG:HG3  | 2:221:B:GLU:HG3  | 2                   | 0.98     | 0.26                | 0.98       |
| (2,1212) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HD2  | 2                   | 0.86     | 0.34                | 0.86       |
| (2,2177) | 2:212:B:ASN:H    | 2:215:B:LYS:HE2  | 2                   | 0.75     | 0.3                 | 0.75       |
| (2,2177) | 2:212:B:ASN:H    | 2:215:B:LYS:HE3  | 2                   | 0.75     | 0.3                 | 0.75       |
| (2,1272) | 1:69:A:GLU:HG2   | 2:219:B:THR:HB   | 2                   | 0.73     | 0.31                | 0.73       |
| (2,2230) | 2:220:B:ARG:HD2  | 2:221:B:GLU:H    | 2                   | 0.69     | 0.09                | 0.69       |
| (2,2230) | 2:220:B:ARG:HD3  | 2:221:B:GLU:H    | 2                   | 0.69     | 0.09                | 0.69       |
| (2,1490) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE2  | 2                   | 0.66     | 0.28                | 0.66       |
| (2,1427) | 2:215:B:LYS:H    | 2:215:B:LYS:HG3  | 2                   | 0.64     | 0.3                 | 0.64       |
| (2,2191) | 2:213:B:PRO:HB2  | 2:214:B:LEU:HD11 | 2                   | 0.64     | 0.3                 | 0.64       |
| (2,2191) | 2:213:B:PRO:HB2  | 2:214:B:LEU:HD12 | 2                   | 0.64     | 0.3                 | 0.64       |
| (2,2191) | 2:213:B:PRO:HB2  | 2:214:B:LEU:HD13 | 2                   | 0.64     | 0.3                 | 0.64       |
| (2,2191) | 2:213:B:PRO:HB2  | 2:214:B:LEU:HD21 | 2                   | 0.64     | 0.3                 | 0.64       |
| (2,2191) | 2:213:B:PRO:HB2  | 2:214:B:LEU:HD22 | 2                   | 0.64     | 0.3                 | 0.64       |
| (2,2191) | 2:213:B:PRO:HB2  | 2:214:B:LEU:HD23 | 2                   | 0.64     | 0.3                 | 0.64       |
| (2,2191) | 2:213:B:PRO:HB3  | 2:214:B:LEU:HD11 | 2                   | 0.64     | 0.3                 | 0.64       |
| (2,2191) | 2:213:B:PRO:HB3  | 2:214:B:LEU:HD12 | 2                   | 0.64     | 0.3                 | 0.64       |
| (2,2191) | 2:213:B:PRO:HB3  | 2:214:B:LEU:HD13 | 2                   | 0.64     | 0.3                 | 0.64       |
| (2,2191) | 2:213:B:PRO:HB3  | 2:214:B:LEU:HD21 | 2                   | 0.64     | 0.3                 | 0.64       |
| (2,2191) | 2:213:B:PRO:HB3  | 2:214:B:LEU:HD22 | 2                   | 0.64     | 0.3                 | 0.64       |
| (2,2191) | 2:213:B:PRO:HB3  | 2:214:B:LEU:HD23 | 2                   | 0.64     | 0.3                 | 0.64       |
| (2,1249) | 1:75:A:GLU:H     | 2:214:B:LEU:HD11 | 2                   | 0.62     | 0.28                | 0.62       |
| (2,1249) | 1:75:A:GLU:H     | 2:214:B:LEU:HD12 | 2                   | 0.62     | 0.28                | 0.62       |
| (2,1249) | 1:75:A:GLU:H     | 2:214:B:LEU:HD13 | 2                   | 0.62     | 0.28                | 0.62       |
| (2,1164) | 1:71:A:GLU:HG3   | 2:217:B:ARG:HB2  | 2                   | 0.6      | 0.05                | 0.6        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1215) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD21 | 2                   | 0.59     | 0.26                | 0.59       |
| (2,1215) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD22 | 2                   | 0.59     | 0.26                | 0.59       |
| (2,1215) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD23 | 2                   | 0.59     | 0.26                | 0.59       |
| (2,1273) | 2:220:B:ARG:HD3  | 2:221:B:GLU:H    | 2                   | 0.53     | 0.06                | 0.53       |
| (2,1319) | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD21 | 2                   | 0.53     | 0.05                | 0.53       |
| (2,1319) | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD22 | 2                   | 0.53     | 0.05                | 0.53       |
| (2,1319) | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD23 | 2                   | 0.53     | 0.05                | 0.53       |
| (2,1171) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HB2  | 2                   | 0.52     | 0.16                | 0.52       |
| (2,1459) | 2:220:B:ARG:HD2  | 2:221:B:GLU:H    | 2                   | 0.52     | 0.15                | 0.52       |
| (2,2202) | 2:215:B:LYS:HB2  | 2:215:B:LYS:HE2  | 2                   | 0.5      | 0.01                | 0.5        |
| (2,2202) | 2:215:B:LYS:HB2  | 2:215:B:LYS:HE3  | 2                   | 0.5      | 0.01                | 0.5        |
| (2,1263) | 2:208:B:GLN:HE21 | 2:219:B:THR:HA   | 2                   | 0.48     | 0.01                | 0.48       |
| (2,1245) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HG3  | 2                   | 0.48     | 0.37                | 0.48       |
| (2,2189) | 2:213:B:PRO:HA   | 2:214:B:LEU:HD11 | 2                   | 0.45     | 0.16                | 0.45       |
| (2,2189) | 2:213:B:PRO:HA   | 2:214:B:LEU:HD12 | 2                   | 0.45     | 0.16                | 0.45       |
| (2,2189) | 2:213:B:PRO:HA   | 2:214:B:LEU:HD13 | 2                   | 0.45     | 0.16                | 0.45       |
| (2,2189) | 2:213:B:PRO:HA   | 2:214:B:LEU:HD21 | 2                   | 0.45     | 0.16                | 0.45       |
| (2,2189) | 2:213:B:PRO:HA   | 2:214:B:LEU:HD22 | 2                   | 0.45     | 0.16                | 0.45       |
| (2,2189) | 2:213:B:PRO:HA   | 2:214:B:LEU:HD23 | 2                   | 0.45     | 0.16                | 0.45       |
| (2,2163) | 2:209:B:ARG:HG2  | 2:210:B:SER:HA   | 2                   | 0.44     | 0.28                | 0.44       |
| (2,2163) | 2:209:B:ARG:HG3  | 2:210:B:SER:HA   | 2                   | 0.44     | 0.28                | 0.44       |
| (2,1248) | 1:74:A:PHE:H     | 2:214:B:LEU:HD11 | 2                   | 0.42     | 0.19                | 0.42       |
| (2,1248) | 1:74:A:PHE:H     | 2:214:B:LEU:HD12 | 2                   | 0.42     | 0.19                | 0.42       |
| (2,1248) | 1:74:A:PHE:H     | 2:214:B:LEU:HD13 | 2                   | 0.42     | 0.19                | 0.42       |
| (2,1393) | 2:206:B:ARG:H    | 2:206:B:ARG:HD2  | 2                   | 0.42     | 0.04                | 0.42       |
| (2,2203) | 2:215:B:LYS:HB3  | 2:215:B:LYS:HE2  | 2                   | 0.4      | 0.0                 | 0.4        |
| (2,2203) | 2:215:B:LYS:HB3  | 2:215:B:LYS:HE3  | 2                   | 0.4      | 0.0                 | 0.4        |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD11 | 2                   | 0.38     | 0.01                | 0.38       |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD12 | 2                   | 0.38     | 0.01                | 0.38       |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD13 | 2                   | 0.38     | 0.01                | 0.38       |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD21 | 2                   | 0.38     | 0.01                | 0.38       |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD22 | 2                   | 0.38     | 0.01                | 0.38       |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD23 | 2                   | 0.38     | 0.01                | 0.38       |
| (2,2105) | 2:206:B:ARG:HB2  | 2:207:B:VAL:H    | 2                   | 0.38     | 0.05                | 0.38       |
| (2,2105) | 2:206:B:ARG:HB3  | 2:207:B:VAL:H    | 2                   | 0.38     | 0.05                | 0.38       |
| (2,1114) | 1:37:A:SER:H     | 2:214:B:LEU:HA   | 2                   | 0.36     | 0.04                | 0.36       |
| (2,1261) | 2:214:B:LEU:HA   | 2:215:B:LYS:HB2  | 2                   | 0.36     | 0.05                | 0.36       |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD11 | 2                   | 0.32     | 0.12                | 0.32       |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD12 | 2                   | 0.32     | 0.12                | 0.32       |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD13 | 2                   | 0.32     | 0.12                | 0.32       |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD21 | 2                   | 0.32     | 0.12                | 0.32       |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD22 | 2                   | 0.32     | 0.12                | 0.32       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD23 | 2                   | 0.32     | 0.12                | 0.32       |
| (2,1396) | 2:205:B:TRP:HB2  | 2:206:B:ARG:H    | 2                   | 0.32     | 0.14                | 0.32       |
| (2,147)  | 1:30:A:TYR:HA    | 2:214:B:LEU:HD21 | 2                   | 0.3      | 0.02                | 0.3        |
| (2,147)  | 1:30:A:TYR:HA    | 2:214:B:LEU:HD22 | 2                   | 0.3      | 0.02                | 0.3        |
| (2,147)  | 1:30:A:TYR:HA    | 2:214:B:LEU:HD23 | 2                   | 0.3      | 0.02                | 0.3        |
| (2,1691) | 1:41:A:ASN:HD21  | 2:207:B:VAL:HB   | 2                   | 0.3      | 0.18                | 0.3        |
| (2,1691) | 1:41:A:ASN:HD22  | 2:207:B:VAL:HB   | 2                   | 0.3      | 0.18                | 0.3        |
| (2,1435) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H    | 2                   | 0.28     | 0.02                | 0.28       |
| (2,1435) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H    | 2                   | 0.28     | 0.02                | 0.28       |
| (2,1435) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H    | 2                   | 0.28     | 0.02                | 0.28       |
| (2,802)  | 1:74:A:PHE:H     | 2:214:B:LEU:HB3  | 2                   | 0.26     | 0.08                | 0.26       |
| (2,1256) | 1:73:A:ASP:HA    | 2:215:B:LYS:HB3  | 2                   | 0.26     | 0.02                | 0.26       |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD11 | 2                   | 0.26     | 0.09                | 0.26       |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD12 | 2                   | 0.26     | 0.09                | 0.26       |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD13 | 2                   | 0.26     | 0.09                | 0.26       |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD21 | 2                   | 0.26     | 0.09                | 0.26       |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD22 | 2                   | 0.26     | 0.09                | 0.26       |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD23 | 2                   | 0.26     | 0.09                | 0.26       |
| (2,1416) | 2:215:B:LYS:H    | 2:215:B:LYS:HB2  | 2                   | 0.26     | 0.05                | 0.26       |
| (2,1131) | 1:72:A:ILE:H     | 2:217:B:ARG:HB2  | 2                   | 0.26     | 0.08                | 0.26       |
| (2,2100) | 2:206:B:ARG:H    | 2:206:B:ARG:HD2  | 2                   | 0.25     | 0.07                | 0.25       |
| (2,2100) | 2:206:B:ARG:H    | 2:206:B:ARG:HD3  | 2                   | 0.25     | 0.07                | 0.25       |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD11 | 2                   | 0.24     | 0.1                 | 0.24       |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD12 | 2                   | 0.24     | 0.1                 | 0.24       |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD13 | 2                   | 0.24     | 0.1                 | 0.24       |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD21 | 2                   | 0.24     | 0.1                 | 0.24       |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD22 | 2                   | 0.24     | 0.1                 | 0.24       |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD23 | 2                   | 0.24     | 0.1                 | 0.24       |
| (2,1428) | 2:208:B:GLN:H    | 2:219:B:THR:HG21 | 2                   | 0.24     | 0.1                 | 0.24       |
| (2,1428) | 2:208:B:GLN:H    | 2:219:B:THR:HG22 | 2                   | 0.24     | 0.1                 | 0.24       |
| (2,1428) | 2:208:B:GLN:H    | 2:219:B:THR:HG23 | 2                   | 0.24     | 0.1                 | 0.24       |
| (2,103)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ2  | 2                   | 0.22     | 0.01                | 0.22       |
| (2,103)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ2  | 2                   | 0.22     | 0.01                | 0.22       |
| (2,103)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ2  | 2                   | 0.22     | 0.01                | 0.22       |
| (2,679)  | 1:34:A:ARG:H     | 2:214:B:LEU:HD11 | 2                   | 0.21     | 0.07                | 0.21       |
| (2,679)  | 1:34:A:ARG:H     | 2:214:B:LEU:HD12 | 2                   | 0.21     | 0.07                | 0.21       |
| (2,679)  | 1:34:A:ARG:H     | 2:214:B:LEU:HD13 | 2                   | 0.21     | 0.07                | 0.21       |
| (2,1481) | 2:212:B:ASN:H    | 2:212:B:ASN:HD22 | 2                   | 0.21     | 0.03                | 0.21       |
| (2,2119) | 2:207:B:VAL:HG11 | 2:208:B:GLN:H    | 2                   | 0.21     | 0.0                 | 0.21       |
| (2,2119) | 2:207:B:VAL:HG12 | 2:208:B:GLN:H    | 2                   | 0.21     | 0.0                 | 0.21       |
| (2,2119) | 2:207:B:VAL:HG13 | 2:208:B:GLN:H    | 2                   | 0.21     | 0.0                 | 0.21       |
| (2,2119) | 2:207:B:VAL:HG21 | 2:208:B:GLN:H    | 2                   | 0.21     | 0.0                 | 0.21       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,2119) | 2:207:B:VAL:HG22 | 2:208:B:GLN:H    | 2                   | 0.21     | 0.0                 | 0.21       |
| (2,2119) | 2:207:B:VAL:HG23 | 2:208:B:GLN:H    | 2                   | 0.21     | 0.0                 | 0.21       |
| (2,407)  | 1:52:A:VAL:HB    | 1:70:A:ILE:HG21  | 2                   | 0.2      | 0.08                | 0.2        |
| (2,407)  | 1:52:A:VAL:HB    | 1:70:A:ILE:HG22  | 2                   | 0.2      | 0.08                | 0.2        |
| (2,407)  | 1:52:A:VAL:HB    | 1:70:A:ILE:HG23  | 2                   | 0.2      | 0.08                | 0.2        |
| (2,1238) | 2:215:B:LYS:HB3  | 2:215:B:LYS:HE3  | 2                   | 0.2      | 0.0                 | 0.2        |
| (2,1161) | 1:68:A:ASP:HB2   | 2:220:B:ARG:HB2  | 2                   | 0.2      | 0.04                | 0.2        |
| (2,1300) | 1:73:A:ASP:HA    | 2:216:B:ILE:HG12 | 2                   | 0.2      | 0.04                | 0.2        |
| (2,2089) | 2:205:B:TRP:HB2  | 2:220:B:ARG:HB2  | 2                   | 0.2      | 0.02                | 0.2        |
| (2,2089) | 2:205:B:TRP:HB2  | 2:220:B:ARG:HB3  | 2                   | 0.2      | 0.02                | 0.2        |
| (2,2032) | 1:87:A:ARG:HD2   | 1:88:A:TYR:HD1   | 2                   | 0.17     | 0.03                | 0.17       |
| (2,2032) | 1:87:A:ARG:HD2   | 1:88:A:TYR:HD2   | 2                   | 0.17     | 0.03                | 0.17       |
| (2,2032) | 1:87:A:ARG:HD3   | 1:88:A:TYR:HD1   | 2                   | 0.17     | 0.03                | 0.17       |
| (2,2032) | 1:87:A:ARG:HD3   | 1:88:A:TYR:HD2   | 2                   | 0.17     | 0.03                | 0.17       |
| (2,1160) | 2:204:B:THR:HA   | 2:205:B:TRP:HB3  | 2                   | 0.16     | 0.01                | 0.16       |
| (2,2068) | 1:95:A:LYS:H     | 1:96:A:LYS:HG2   | 2                   | 0.16     | 0.05                | 0.16       |
| (2,2068) | 1:95:A:LYS:H     | 1:96:A:LYS:HG3   | 2                   | 0.16     | 0.05                | 0.16       |
| (2,1728) | 1:48:A:LEU:HB2   | 2:205:B:TRP:HE1  | 2                   | 0.15     | 0.02                | 0.15       |
| (2,1728) | 1:48:A:LEU:HB3   | 2:205:B:TRP:HE1  | 2                   | 0.15     | 0.02                | 0.15       |
| (2,2081) | 2:203:B:LEU:HD11 | 2:204:B:THR:H    | 2                   | 0.15     | 0.02                | 0.15       |
| (2,2081) | 2:203:B:LEU:HD12 | 2:204:B:THR:H    | 2                   | 0.15     | 0.02                | 0.15       |
| (2,2081) | 2:203:B:LEU:HD13 | 2:204:B:THR:H    | 2                   | 0.15     | 0.02                | 0.15       |
| (2,2081) | 2:203:B:LEU:HD21 | 2:204:B:THR:H    | 2                   | 0.15     | 0.02                | 0.15       |
| (2,2081) | 2:203:B:LEU:HD22 | 2:204:B:THR:H    | 2                   | 0.15     | 0.02                | 0.15       |
| (2,2081) | 2:203:B:LEU:HD23 | 2:204:B:THR:H    | 2                   | 0.15     | 0.02                | 0.15       |
| (2,1280) | 1:72:A:ILE:HG21  | 2:216:B:ILE:HB   | 2                   | 0.15     | 0.0                 | 0.15       |
| (2,1280) | 1:72:A:ILE:HG22  | 2:216:B:ILE:HB   | 2                   | 0.15     | 0.0                 | 0.15       |
| (2,1280) | 1:72:A:ILE:HG23  | 2:216:B:ILE:HB   | 2                   | 0.15     | 0.0                 | 0.15       |
| (2,1287) | 1:48:A:LEU:HA    | 2:218:B:LEU:HG   | 2                   | 0.15     | 0.0                 | 0.15       |
| (2,1612) | 1:35:A:GLN:HA    | 1:39:A:ASP:HB2   | 2                   | 0.15     | 0.0                 | 0.15       |
| (2,1612) | 1:35:A:GLN:HA    | 1:39:A:ASP:HB3   | 2                   | 0.15     | 0.0                 | 0.15       |
| (2,568)  | 1:28:A:MET:HE1   | 1:82:A:LEU:H     | 2                   | 0.14     | 0.04                | 0.14       |
| (2,568)  | 1:28:A:MET:HE2   | 1:82:A:LEU:H     | 2                   | 0.14     | 0.04                | 0.14       |
| (2,568)  | 1:28:A:MET:HE3   | 1:82:A:LEU:H     | 2                   | 0.14     | 0.04                | 0.14       |
| (2,1236) | 2:215:B:LYS:HB3  | 2:215:B:LYS:HE2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,1609) | 1:35:A:GLN:H     | 1:38:A:LEU:HD11  | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,1609) | 1:35:A:GLN:H     | 1:38:A:LEU:HD12  | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,1609) | 1:35:A:GLN:H     | 1:38:A:LEU:HD13  | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,1609) | 1:35:A:GLN:H     | 1:38:A:LEU:HD21  | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,1609) | 1:35:A:GLN:H     | 1:38:A:LEU:HD22  | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,1609) | 1:35:A:GLN:H     | 1:38:A:LEU:HD23  | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,496)  | 1:71:A:GLU:HG2   | 1:72:A:ILE:H     | 2                   | 0.11     | 0.01                | 0.11       |

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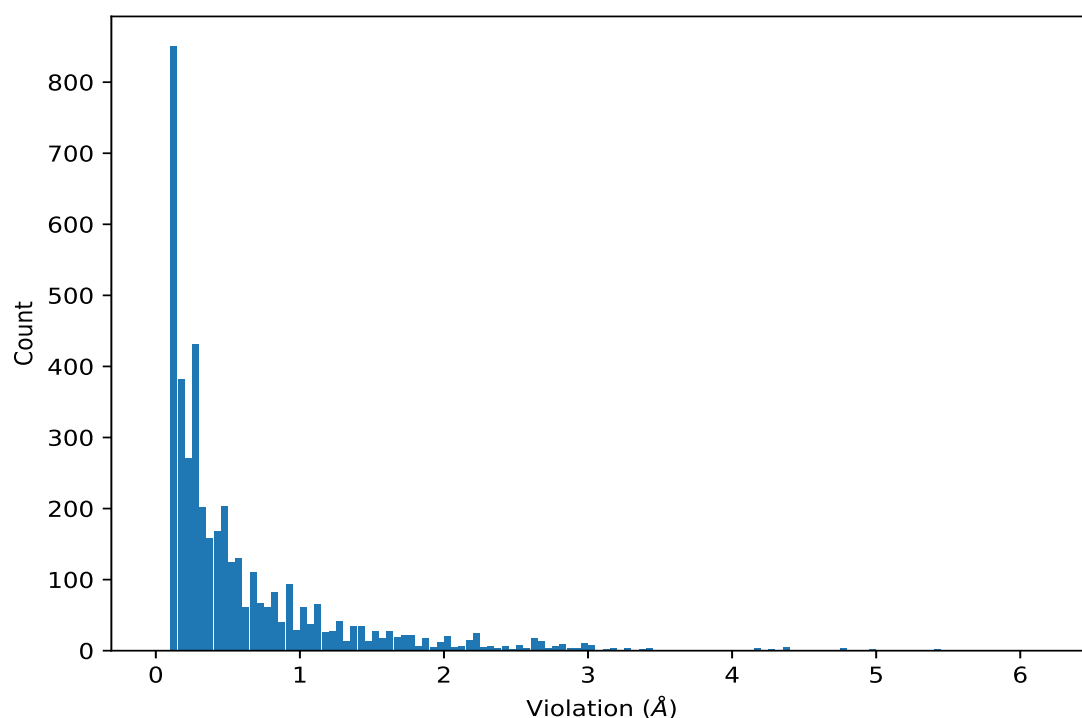
| Key      | Atom-1         | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|------------------|---------------------|----------|---------------------|------------|
| (2,1686) | 1:41:A:ASN:HA  | 2:207:B:VAL:HG11 | 2                   | 0.11     | 0.01                | 0.11       |
| (2,1686) | 1:41:A:ASN:HA  | 2:207:B:VAL:HG12 | 2                   | 0.11     | 0.01                | 0.11       |
| (2,1686) | 1:41:A:ASN:HA  | 2:207:B:VAL:HG13 | 2                   | 0.11     | 0.01                | 0.11       |
| (2,1686) | 1:41:A:ASN:HA  | 2:207:B:VAL:HG21 | 2                   | 0.11     | 0.01                | 0.11       |
| (2,1686) | 1:41:A:ASN:HA  | 2:207:B:VAL:HG22 | 2                   | 0.11     | 0.01                | 0.11       |
| (2,1686) | 1:41:A:ASN:HA  | 2:207:B:VAL:HG23 | 2                   | 0.11     | 0.01                | 0.11       |
| (2,1926) | 1:73:A:ASP:HB2 | 1:76:A:THR:HG21  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,1926) | 1:73:A:ASP:HB2 | 1:76:A:THR:HG22  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,1926) | 1:73:A:ASP:HB2 | 1:76:A:THR:HG23  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,1926) | 1:73:A:ASP:HB3 | 1:76:A:THR:HG21  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,1926) | 1:73:A:ASP:HB3 | 1:76:A:THR:HG22  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,1926) | 1:73:A:ASP:HB3 | 1:76:A:THR:HG23  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,1953) | 1:75:A:GLU:HB3 | 2:214:B:LEU:HD11 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,1953) | 1:75:A:GLU:HB3 | 2:214:B:LEU:HD12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,1953) | 1:75:A:GLU:HB3 | 2:214:B:LEU:HD13 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,1953) | 1:75:A:GLU:HB3 | 2:214:B:LEU:HD21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,1953) | 1:75:A:GLU:HB3 | 2:214:B:LEU:HD22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,1953) | 1:75:A:GLU:HB3 | 2:214:B:LEU:HD23 | 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 ⓘ

### 9.5.1 Histogram : Distribution of distance violations ⓘ

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) |
|----------|-----------------|-----------------|----------|---------------|
| (2,28)   | 1:69:A:GLU:HA   | 2:205:B:TRP:HZ3 | 4        | 6.16          |
| (2,991)  | 1:70:A:ILE:H    | 2:205:B:TRP:HZ3 | 4        | 5.9           |
| (2,991)  | 1:70:A:ILE:H    | 2:205:B:TRP:HZ3 | 3        | 5.72          |
| (2,28)   | 1:69:A:GLU:HA   | 2:205:B:TRP:HZ3 | 3        | 5.44          |
| (2,189)  | 1:70:A:ILE:HG12 | 2:205:B:TRP:HH2 | 3        | 5.41          |
| (2,28)   | 1:69:A:GLU:HA   | 2:205:B:TRP:HZ3 | 17       | 5.2           |
| (2,1251) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HG  | 3        | 4.99          |
| (2,13)   | 1:70:A:ILE:HG12 | 2:205:B:TRP:HZ3 | 3        | 4.99          |
| (2,1144) | 2:205:B:TRP:HZ3 | 2:219:B:THR:HA  | 4        | 4.94          |
| (2,28)   | 1:69:A:GLU:HA   | 2:205:B:TRP:HZ3 | 8        | 4.86          |
| (2,991)  | 1:70:A:ILE:H    | 2:205:B:TRP:HZ3 | 8        | 4.78          |
| (2,189)  | 1:70:A:ILE:HG12 | 2:205:B:TRP:HH2 | 4        | 4.76          |
| (2,28)   | 1:69:A:GLU:HA   | 2:205:B:TRP:HZ3 | 13       | 4.75          |
| (2,991)  | 1:70:A:ILE:H    | 2:205:B:TRP:HZ3 | 17       | 4.7           |
| (2,143)  | 1:70:A:ILE:HG13 | 2:205:B:TRP:HH2 | 3        | 4.66          |
| (2,650)  | 1:70:A:ILE:HB   | 2:205:B:TRP:HZ3 | 3        | 4.6           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1144) | 2:205:B:TRP:HZ3 | 2:219:B:THR:HA  | 3        | 4.5           |
| (2,13)   | 1:70:A:ILE:HG12 | 2:205:B:TRP:HZ3 | 4        | 4.41          |
| (2,28)   | 1:69:A:GLU:HA   | 2:205:B:TRP:HZ3 | 19       | 4.39          |
| (2,1251) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HG  | 4        | 4.38          |
| (2,28)   | 1:69:A:GLU:HA   | 2:205:B:TRP:HZ3 | 18       | 4.38          |
| (2,650)  | 1:70:A:ILE:HB   | 2:205:B:TRP:HZ3 | 4        | 4.37          |
| (2,990)  | 1:69:A:GLU:H    | 2:205:B:TRP:HZ3 | 4        | 4.36          |
| (2,1127) | 1:70:A:ILE:H    | 2:205:B:TRP:HH2 | 4        | 4.35          |
| (2,143)  | 1:70:A:ILE:HG13 | 2:205:B:TRP:HH2 | 4        | 4.28          |
| (2,1127) | 1:70:A:ILE:H    | 2:205:B:TRP:HH2 | 3        | 4.27          |
| (2,991)  | 1:70:A:ILE:H    | 2:205:B:TRP:HZ3 | 18       | 4.18          |
| (2,991)  | 1:70:A:ILE:H    | 2:205:B:TRP:HZ3 | 19       | 4.18          |
| (2,990)  | 1:69:A:GLU:H    | 2:205:B:TRP:HZ3 | 3        | 4.17          |
| (2,15)   | 1:70:A:ILE:HG13 | 2:205:B:TRP:HZ3 | 3        | 4.12          |
| (2,1251) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HG  | 19       | 4.07          |
| (2,991)  | 1:70:A:ILE:H    | 2:205:B:TRP:HZ3 | 13       | 4.02          |
| (2,189)  | 1:70:A:ILE:HG12 | 2:205:B:TRP:HH2 | 8        | 3.86          |
| (2,15)   | 1:70:A:ILE:HG13 | 2:205:B:TRP:HZ3 | 4        | 3.8           |
| (2,1144) | 2:205:B:TRP:HZ3 | 2:219:B:THR:HA  | 13       | 3.56          |
| (2,1144) | 2:205:B:TRP:HZ3 | 2:219:B:THR:HA  | 18       | 3.51          |
| (2,1340) | 2:205:B:TRP:HE3 | 2:219:B:THR:H   | 4        | 3.47          |
| (2,1144) | 2:205:B:TRP:HZ3 | 2:219:B:THR:HA  | 8        | 3.44          |
| (2,1127) | 1:70:A:ILE:H    | 2:205:B:TRP:HH2 | 8        | 3.43          |
| (2,208)  | 1:69:A:GLU:HA   | 2:205:B:TRP:HE3 | 4        | 3.41          |
| (2,1251) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HG  | 17       | 3.37          |
| (2,13)   | 1:70:A:ILE:HG12 | 2:205:B:TRP:HZ3 | 8        | 3.37          |
| (2,189)  | 1:70:A:ILE:HG12 | 2:205:B:TRP:HH2 | 18       | 3.32          |
| (2,1340) | 2:205:B:TRP:HE3 | 2:219:B:THR:H   | 3        | 3.29          |
| (2,208)  | 1:69:A:GLU:HA   | 2:205:B:TRP:HE3 | 17       | 3.29          |
| (2,1145) | 2:205:B:TRP:HE3 | 2:219:B:THR:HA  | 4        | 3.27          |
| (2,1144) | 2:205:B:TRP:HZ3 | 2:219:B:THR:HA  | 19       | 3.26          |
| (2,1144) | 2:205:B:TRP:HZ3 | 2:219:B:THR:HA  | 17       | 3.21          |
| (2,1163) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HB3 | 18       | 3.19          |
| (2,1251) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HG  | 20       | 3.18          |
| (2,143)  | 1:70:A:ILE:HG13 | 2:205:B:TRP:HH2 | 8        | 3.17          |
| (2,991)  | 1:70:A:ILE:H    | 2:205:B:TRP:HZ3 | 15       | 3.15          |
| (2,990)  | 1:69:A:GLU:H    | 2:205:B:TRP:HZ3 | 17       | 3.1           |
| (2,1163) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HB3 | 3        | 3.05          |
| (2,650)  | 1:70:A:ILE:HB   | 2:205:B:TRP:HZ3 | 18       | 3.05          |
| (2,100)  | 1:52:A:VAL:HG11 | 2:205:B:TRP:HH2 | 3        | 3.05          |
| (2,100)  | 1:52:A:VAL:HG12 | 2:205:B:TRP:HH2 | 3        | 3.05          |
| (2,100)  | 1:52:A:VAL:HG13 | 2:205:B:TRP:HH2 | 3        | 3.05          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,990)  | 1:69:A:GLU:H    | 2:205:B:TRP:HZ3  | 13       | 3.03          |
| (2,28)   | 1:69:A:GLU:HA   | 2:205:B:TRP:HZ3  | 20       | 3.03          |
| (2,16)   | 2:205:B:TRP:HZ3 | 2:218:B:LEU:HB3  | 4        | 3.0           |
| (2,1163) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HB3  | 4        | 2.99          |
| (2,16)   | 2:205:B:TRP:HZ3 | 2:218:B:LEU:HB3  | 3        | 2.99          |
| (2,990)  | 1:69:A:GLU:H    | 2:205:B:TRP:HZ3  | 8        | 2.98          |
| (2,100)  | 1:52:A:VAL:HG11 | 2:205:B:TRP:HH2  | 4        | 2.96          |
| (2,100)  | 1:52:A:VAL:HG12 | 2:205:B:TRP:HH2  | 4        | 2.96          |
| (2,100)  | 1:52:A:VAL:HG13 | 2:205:B:TRP:HH2  | 4        | 2.96          |
| (2,58)   | 1:76:A:THR:HG21 | 2:215:B:LYS:HG3  | 10       | 2.96          |
| (2,58)   | 1:76:A:THR:HG22 | 2:215:B:LYS:HG3  | 10       | 2.96          |
| (2,58)   | 1:76:A:THR:HG23 | 2:215:B:LYS:HG3  | 10       | 2.96          |
| (2,16)   | 2:205:B:TRP:HZ3 | 2:218:B:LEU:HB3  | 18       | 2.96          |
| (2,13)   | 1:70:A:ILE:HG12 | 2:205:B:TRP:HZ3  | 19       | 2.94          |
| (2,13)   | 1:70:A:ILE:HG12 | 2:205:B:TRP:HZ3  | 17       | 2.93          |
| (2,189)  | 1:70:A:ILE:HG12 | 2:205:B:TRP:HH2  | 19       | 2.92          |
| (2,1251) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HG   | 8        | 2.91          |
| (2,1127) | 1:70:A:ILE:H    | 2:205:B:TRP:HH2  | 18       | 2.9           |
| (2,13)   | 1:70:A:ILE:HG12 | 2:205:B:TRP:HZ3  | 15       | 2.89          |
| (2,650)  | 1:70:A:ILE:HB   | 2:205:B:TRP:HZ3  | 8        | 2.88          |
| (2,1144) | 2:205:B:TRP:HZ3 | 2:219:B:THR:HA   | 11       | 2.85          |
| (2,1145) | 2:205:B:TRP:HE3 | 2:219:B:THR:HA   | 3        | 2.84          |
| (2,13)   | 1:70:A:ILE:HG12 | 2:205:B:TRP:HZ3  | 18       | 2.83          |
| (2,991)  | 1:70:A:ILE:H    | 2:205:B:TRP:HZ3  | 20       | 2.82          |
| (2,531)  | 1:76:A:THR:HG21 | 2:215:B:LYS:HD3  | 10       | 2.82          |
| (2,531)  | 1:76:A:THR:HG22 | 2:215:B:LYS:HD3  | 10       | 2.82          |
| (2,531)  | 1:76:A:THR:HG23 | 2:215:B:LYS:HD3  | 10       | 2.82          |
| (2,1144) | 2:205:B:TRP:HZ3 | 2:219:B:THR:HA   | 15       | 2.81          |
| (2,990)  | 1:69:A:GLU:H    | 2:205:B:TRP:HZ3  | 19       | 2.81          |
| (2,76)   | 1:75:A:GLU:HG3  | 2:214:B:LEU:HB2  | 9        | 2.81          |
| (2,1174) | 2:212:B:ASN:HB2 | 2:215:B:LYS:HB2  | 10       | 2.78          |
| (2,531)  | 1:76:A:THR:HG21 | 2:215:B:LYS:HD3  | 12       | 2.77          |
| (2,531)  | 1:76:A:THR:HG22 | 2:215:B:LYS:HD3  | 12       | 2.77          |
| (2,531)  | 1:76:A:THR:HG23 | 2:215:B:LYS:HD3  | 12       | 2.77          |
| (2,208)  | 1:69:A:GLU:HA   | 2:205:B:TRP:HE3  | 3        | 2.76          |
| (2,143)  | 1:70:A:ILE:HG13 | 2:205:B:TRP:HH2  | 18       | 2.76          |
| (2,28)   | 1:69:A:GLU:HA   | 2:205:B:TRP:HZ3  | 2        | 2.75          |
| (2,990)  | 1:69:A:GLU:H    | 2:205:B:TRP:HZ3  | 18       | 2.73          |
| (2,1340) | 2:205:B:TRP:HE3 | 2:219:B:THR:H    | 17       | 2.7           |
| (2,12)   | 2:204:B:THR:HB  | 2:205:B:TRP:HD1  | 17       | 2.7           |
| (2,2192) | 2:213:B:PRO:HG2 | 2:214:B:LEU:HD11 | 9        | 2.69          |
| (2,2192) | 2:213:B:PRO:HG2 | 2:214:B:LEU:HD12 | 9        | 2.69          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2192) | 2:213:B:PRO:HG2 | 2:214:B:LEU:HD13 | 9        | 2.69          |
| (2,2192) | 2:213:B:PRO:HG2 | 2:214:B:LEU:HD21 | 9        | 2.69          |
| (2,2192) | 2:213:B:PRO:HG2 | 2:214:B:LEU:HD22 | 9        | 2.69          |
| (2,2192) | 2:213:B:PRO:HG2 | 2:214:B:LEU:HD23 | 9        | 2.69          |
| (2,1606) | 1:34:A:ARG:HD2  | 2:213:B:PRO:HG3  | 13       | 2.69          |
| (2,1606) | 1:34:A:ARG:HD3  | 2:213:B:PRO:HG3  | 13       | 2.69          |
| (2,162)  | 1:52:A:VAL:HG11 | 2:205:B:TRP:HZ3  | 4        | 2.68          |
| (2,162)  | 1:52:A:VAL:HG12 | 2:205:B:TRP:HZ3  | 4        | 2.68          |
| (2,162)  | 1:52:A:VAL:HG13 | 2:205:B:TRP:HZ3  | 4        | 2.68          |
| (2,1231) | 2:205:B:TRP:HE3 | 2:218:B:LEU:HA   | 4        | 2.67          |
| (2,1340) | 2:205:B:TRP:HE3 | 2:219:B:THR:H    | 18       | 2.66          |
| (2,531)  | 1:76:A:THR:HG21 | 2:215:B:LYS:HD3  | 2        | 2.64          |
| (2,531)  | 1:76:A:THR:HG22 | 2:215:B:LYS:HD3  | 2        | 2.64          |
| (2,531)  | 1:76:A:THR:HG23 | 2:215:B:LYS:HD3  | 2        | 2.64          |
| (2,100)  | 1:52:A:VAL:HG11 | 2:205:B:TRP:HH2  | 18       | 2.64          |
| (2,100)  | 1:52:A:VAL:HG12 | 2:205:B:TRP:HH2  | 18       | 2.64          |
| (2,100)  | 1:52:A:VAL:HG13 | 2:205:B:TRP:HH2  | 18       | 2.64          |
| (2,58)   | 1:76:A:THR:HG21 | 2:215:B:LYS:HG3  | 2        | 2.63          |
| (2,58)   | 1:76:A:THR:HG22 | 2:215:B:LYS:HG3  | 2        | 2.63          |
| (2,58)   | 1:76:A:THR:HG23 | 2:215:B:LYS:HG3  | 2        | 2.63          |
| (2,162)  | 1:52:A:VAL:HG11 | 2:205:B:TRP:HZ3  | 3        | 2.62          |
| (2,162)  | 1:52:A:VAL:HG12 | 2:205:B:TRP:HZ3  | 3        | 2.62          |
| (2,162)  | 1:52:A:VAL:HG13 | 2:205:B:TRP:HZ3  | 3        | 2.62          |
| (2,1218) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD21 | 9        | 2.61          |
| (2,1218) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD22 | 9        | 2.61          |
| (2,1218) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD23 | 9        | 2.61          |
| (2,208)  | 1:69:A:GLU:HA   | 2:205:B:TRP:HE3  | 8        | 2.61          |
| (2,1231) | 2:205:B:TRP:HE3 | 2:218:B:LEU:HA   | 3        | 2.6           |
| (2,650)  | 1:70:A:ILE:HB   | 2:205:B:TRP:HZ3  | 19       | 2.59          |
| (2,2149) | 2:208:B:GLN:HG2 | 2:217:B:ARG:HG2  | 20       | 2.57          |
| (2,2149) | 2:208:B:GLN:HG3 | 2:217:B:ARG:HG2  | 20       | 2.57          |
| (2,615)  | 1:75:A:GLU:HG2  | 2:214:B:LEU:HB2  | 9        | 2.56          |
| (2,1251) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HG   | 11       | 2.55          |
| (2,1334) | 1:34:A:ARG:HG3  | 2:213:B:PRO:HG3  | 13       | 2.54          |
| (2,1144) | 2:205:B:TRP:HZ3 | 2:219:B:THR:HA   | 2        | 2.54          |
| (2,650)  | 1:70:A:ILE:HB   | 2:205:B:TRP:HZ3  | 17       | 2.54          |
| (2,12)   | 2:204:B:THR:HB  | 2:205:B:TRP:HD1  | 3        | 2.54          |
| (2,1251) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HG   | 12       | 2.51          |
| (2,15)   | 1:70:A:ILE:HG13 | 2:205:B:TRP:HZ3  | 8        | 2.51          |
| (2,208)  | 1:69:A:GLU:HA   | 2:205:B:TRP:HE3  | 13       | 2.5           |
| (2,28)   | 1:69:A:GLU:HA   | 2:205:B:TRP:HZ3  | 15       | 2.46          |
| (2,15)   | 1:70:A:ILE:HG13 | 2:205:B:TRP:HZ3  | 17       | 2.45          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,23)   | 1:70:A:ILE:HD11 | 2:205:B:TRP:HH2  | 3        | 2.43          |
| (2,23)   | 1:70:A:ILE:HD12 | 2:205:B:TRP:HH2  | 3        | 2.43          |
| (2,23)   | 1:70:A:ILE:HD13 | 2:205:B:TRP:HH2  | 3        | 2.43          |
| (2,1175) | 2:210:B:SER:HB3 | 2:215:B:LYS:HB3  | 2        | 2.42          |
| (2,1127) | 1:70:A:ILE:H    | 2:205:B:TRP:HH2  | 19       | 2.42          |
| (2,143)  | 1:70:A:ILE:HG13 | 2:205:B:TRP:HH2  | 19       | 2.42          |
| (2,3)    | 2:205:B:TRP:HE3 | 2:218:B:LEU:HB3  | 18       | 2.41          |
| (2,1334) | 1:34:A:ARG:HG3  | 2:213:B:PRO:HG3  | 6        | 2.39          |
| (2,1144) | 2:205:B:TRP:HZ3 | 2:219:B:THR:HA   | 20       | 2.39          |
| (2,189)  | 1:70:A:ILE:HG12 | 2:205:B:TRP:HH2  | 15       | 2.37          |
| (2,189)  | 1:70:A:ILE:HG12 | 2:205:B:TRP:HH2  | 17       | 2.36          |
| (2,1231) | 2:205:B:TRP:HE3 | 2:218:B:LEU:HA   | 17       | 2.33          |
| (2,189)  | 1:70:A:ILE:HG12 | 2:205:B:TRP:HH2  | 13       | 2.32          |
| (2,1340) | 2:205:B:TRP:HE3 | 2:219:B:THR:H    | 19       | 2.31          |
| (2,1251) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HG   | 13       | 2.31          |
| (2,1127) | 1:70:A:ILE:H    | 2:205:B:TRP:HH2  | 17       | 2.31          |
| (2,650)  | 1:70:A:ILE:HB   | 2:205:B:TRP:HZ3  | 15       | 2.31          |
| (2,801)  | 1:74:A:PHE:H    | 2:214:B:LEU:HB2  | 9        | 2.3           |
| (2,1340) | 2:205:B:TRP:HE3 | 2:219:B:THR:H    | 13       | 2.29          |
| (2,1127) | 1:70:A:ILE:H    | 2:205:B:TRP:HH2  | 13       | 2.28          |
| (2,1602) | 1:34:A:ARG:HG3  | 2:213:B:PRO:HB2  | 15       | 2.26          |
| (2,1602) | 1:34:A:ARG:HG3  | 2:213:B:PRO:HB3  | 15       | 2.26          |
| (2,2193) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD11 | 9        | 2.24          |
| (2,2193) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD12 | 9        | 2.24          |
| (2,2193) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD13 | 9        | 2.24          |
| (2,2193) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD21 | 9        | 2.24          |
| (2,2193) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD22 | 9        | 2.24          |
| (2,2193) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD23 | 9        | 2.24          |
| (2,803)  | 1:75:A:GLU:H    | 2:214:B:LEU:HB2  | 9        | 2.24          |
| (2,991)  | 1:70:A:ILE:H    | 2:205:B:TRP:HZ3  | 11       | 2.22          |
| (2,162)  | 1:52:A:VAL:HG11 | 2:205:B:TRP:HZ3  | 18       | 2.22          |
| (2,162)  | 1:52:A:VAL:HG12 | 2:205:B:TRP:HZ3  | 18       | 2.22          |
| (2,162)  | 1:52:A:VAL:HG13 | 2:205:B:TRP:HZ3  | 18       | 2.22          |
| (2,100)  | 1:52:A:VAL:HG11 | 2:205:B:TRP:HH2  | 8        | 2.22          |
| (2,100)  | 1:52:A:VAL:HG12 | 2:205:B:TRP:HH2  | 8        | 2.22          |
| (2,100)  | 1:52:A:VAL:HG13 | 2:205:B:TRP:HH2  | 8        | 2.22          |
| (2,58)   | 1:76:A:THR:HG21 | 2:215:B:LYS:HG3  | 11       | 2.22          |
| (2,58)   | 1:76:A:THR:HG22 | 2:215:B:LYS:HG3  | 11       | 2.22          |
| (2,58)   | 1:76:A:THR:HG23 | 2:215:B:LYS:HG3  | 11       | 2.22          |
| (2,16)   | 2:205:B:TRP:HZ3 | 2:218:B:LEU:HB3  | 19       | 2.22          |
| (2,15)   | 1:70:A:ILE:HG13 | 2:205:B:TRP:HZ3  | 19       | 2.21          |
| (2,2150) | 2:208:B:GLN:HG2 | 2:217:B:ARG:HG3  | 20       | 2.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2150) | 2:208:B:GLN:HG3 | 2:217:B:ARG:HG3  | 20       | 2.2           |
| (2,58)   | 1:76:A:THR:HG21 | 2:215:B:LYS:HG3  | 20       | 2.2           |
| (2,58)   | 1:76:A:THR:HG22 | 2:215:B:LYS:HG3  | 20       | 2.2           |
| (2,58)   | 1:76:A:THR:HG23 | 2:215:B:LYS:HG3  | 20       | 2.2           |
| (2,1606) | 1:34:A:ARG:HD2  | 2:213:B:PRO:HG3  | 6        | 2.19          |
| (2,1606) | 1:34:A:ARG:HD3  | 2:213:B:PRO:HG3  | 6        | 2.19          |
| (2,1126) | 1:70:A:ILE:H    | 2:205:B:TRP:HE3  | 4        | 2.19          |
| (2,14)   | 1:70:A:ILE:HD11 | 2:205:B:TRP:HZ3  | 3        | 2.18          |
| (2,14)   | 1:70:A:ILE:HD12 | 2:205:B:TRP:HZ3  | 3        | 2.18          |
| (2,14)   | 1:70:A:ILE:HD13 | 2:205:B:TRP:HZ3  | 3        | 2.18          |
| (2,2149) | 2:208:B:GLN:HG2 | 2:217:B:ARG:HG2  | 2        | 2.17          |
| (2,2149) | 2:208:B:GLN:HG3 | 2:217:B:ARG:HG2  | 2        | 2.17          |
| (2,16)   | 2:205:B:TRP:HZ3 | 2:218:B:LEU:HB3  | 17       | 2.17          |
| (2,2151) | 2:208:B:GLN:HG2 | 2:217:B:ARG:HD2  | 20       | 2.16          |
| (2,2151) | 2:208:B:GLN:HG2 | 2:217:B:ARG:HD3  | 20       | 2.16          |
| (2,2151) | 2:208:B:GLN:HG3 | 2:217:B:ARG:HD2  | 20       | 2.16          |
| (2,2151) | 2:208:B:GLN:HG3 | 2:217:B:ARG:HD3  | 20       | 2.16          |
| (2,1145) | 2:205:B:TRP:HE3 | 2:219:B:THR:HA   | 17       | 2.16          |
| (2,1145) | 2:205:B:TRP:HE3 | 2:219:B:THR:HA   | 13       | 2.15          |
| (2,143)  | 1:70:A:ILE:HG13 | 2:205:B:TRP:HH2  | 17       | 2.13          |
| (2,1340) | 2:205:B:TRP:HE3 | 2:219:B:THR:H    | 15       | 2.12          |
| (2,991)  | 1:70:A:ILE:H    | 2:205:B:TRP:HZ3  | 2        | 2.12          |
| (2,12)   | 2:204:B:THR:HB  | 2:205:B:TRP:HD1  | 4        | 2.12          |
| (2,1340) | 2:205:B:TRP:HE3 | 2:219:B:THR:H    | 11       | 2.1           |
| (2,15)   | 1:70:A:ILE:HG13 | 2:205:B:TRP:HZ3  | 18       | 2.1           |
| (2,1231) | 2:205:B:TRP:HE3 | 2:218:B:LEU:HA   | 18       | 2.09          |
| (2,650)  | 1:70:A:ILE:HB   | 2:205:B:TRP:HZ3  | 13       | 2.08          |
| (2,13)   | 1:70:A:ILE:HG12 | 2:205:B:TRP:HZ3  | 13       | 2.08          |
| (2,143)  | 1:70:A:ILE:HG13 | 2:205:B:TRP:HH2  | 13       | 2.06          |
| (2,3)    | 2:205:B:TRP:HE3 | 2:218:B:LEU:HB3  | 4        | 2.06          |
| (2,1126) | 1:70:A:ILE:H    | 2:205:B:TRP:HE3  | 3        | 2.05          |
| (2,1145) | 2:205:B:TRP:HE3 | 2:219:B:THR:HA   | 8        | 2.03          |
| (2,1145) | 2:205:B:TRP:HE3 | 2:219:B:THR:HA   | 18       | 2.03          |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD11 | 3        | 2.02          |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD12 | 3        | 2.02          |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD13 | 3        | 2.02          |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD21 | 3        | 2.02          |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD22 | 3        | 2.02          |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD23 | 3        | 2.02          |
| (2,2192) | 2:213:B:PRO:HG2 | 2:214:B:LEU:HD11 | 3        | 2.01          |
| (2,2192) | 2:213:B:PRO:HG2 | 2:214:B:LEU:HD12 | 3        | 2.01          |
| (2,2192) | 2:213:B:PRO:HG2 | 2:214:B:LEU:HD13 | 3        | 2.01          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD21 | 3        | 2.01          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD22 | 3        | 2.01          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD23 | 3        | 2.01          |
| (2,2149) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG2  | 9        | 2.01          |
| (2,2149) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG2  | 9        | 2.01          |
| (2,3)    | 2:205:B:TRP:HE3  | 2:218:B:LEU:HB3  | 3        | 2.01          |
| (2,1163) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HB3  | 19       | 2.0           |
| (2,208)  | 1:69:A:GLU:HA    | 2:205:B:TRP:HE3  | 18       | 2.0           |
| (2,1144) | 2:205:B:TRP:HZ3  | 2:219:B:THR:HA   | 5        | 1.98          |
| (2,208)  | 1:69:A:GLU:HA    | 2:205:B:TRP:HE3  | 19       | 1.98          |
| (2,2200) | 2:214:B:LEU:HD11 | 2:215:B:LYS:HG3  | 12       | 1.97          |
| (2,2200) | 2:214:B:LEU:HD12 | 2:215:B:LYS:HG3  | 12       | 1.97          |
| (2,2200) | 2:214:B:LEU:HD13 | 2:215:B:LYS:HG3  | 12       | 1.97          |
| (2,2200) | 2:214:B:LEU:HD21 | 2:215:B:LYS:HG3  | 12       | 1.97          |
| (2,2200) | 2:214:B:LEU:HD22 | 2:215:B:LYS:HG3  | 12       | 1.97          |
| (2,2200) | 2:214:B:LEU:HD23 | 2:215:B:LYS:HG3  | 12       | 1.97          |
| (2,531)  | 1:76:A:THR:HG21  | 2:215:B:LYS:HD3  | 18       | 1.97          |
| (2,531)  | 1:76:A:THR:HG22  | 2:215:B:LYS:HD3  | 18       | 1.97          |
| (2,531)  | 1:76:A:THR:HG23  | 2:215:B:LYS:HD3  | 18       | 1.97          |
| (2,1334) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HG3  | 9        | 1.96          |
| (2,1126) | 1:70:A:ILE:H     | 2:205:B:TRP:HE3  | 17       | 1.95          |
| (2,1231) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HA   | 19       | 1.91          |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3  | 14       | 1.91          |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3  | 14       | 1.91          |
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3  | 14       | 1.91          |
| (2,2150) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG3  | 2        | 1.9           |
| (2,2150) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG3  | 2        | 1.9           |
| (2,1340) | 2:205:B:TRP:HE3  | 2:219:B:THR:H    | 8        | 1.9           |
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 9        | 1.89          |
| (2,1251) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HG   | 15       | 1.89          |
| (2,11)   | 2:204:B:THR:HA   | 2:205:B:TRP:HD1  | 4        | 1.89          |
| (2,3)    | 2:205:B:TRP:HE3  | 2:218:B:LEU:HB3  | 17       | 1.89          |
| (2,1237) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB2  | 2        | 1.88          |
| (2,162)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ3  | 8        | 1.87          |
| (2,162)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ3  | 8        | 1.87          |
| (2,162)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ3  | 8        | 1.87          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 8        | 1.87          |
| (2,2150) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG3  | 9        | 1.86          |
| (2,2150) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG3  | 9        | 1.86          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 13       | 1.86          |
| (2,23)   | 1:70:A:ILE:HD11  | 2:205:B:TRP:HH2  | 4        | 1.85          |
| (2,23)   | 1:70:A:ILE:HD12  | 2:205:B:TRP:HH2  | 4        | 1.85          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,23)   | 1:70:A:ILE:HD13  | 2:205:B:TRP:HH2  | 4        | 1.85          |
| (2,1340) | 2:205:B:TRP:HE3  | 2:219:B:THR:H    | 20       | 1.84          |
| (2,1144) | 2:205:B:TRP:HZ3  | 2:219:B:THR:HA   | 6        | 1.83          |
| (2,1251) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HG   | 2        | 1.82          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 19       | 1.82          |
| (2,1144) | 2:205:B:TRP:HZ3  | 2:219:B:THR:HA   | 12       | 1.81          |
| (2,1163) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HB3  | 8        | 1.8           |
| (2,28)   | 1:69:A:GLU:HA    | 2:205:B:TRP:HZ3  | 6        | 1.8           |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 2        | 1.79          |
| (2,1794) | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ3  | 4        | 1.78          |
| (2,1794) | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ3  | 4        | 1.78          |
| (2,1794) | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ3  | 4        | 1.78          |
| (2,1794) | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ3  | 4        | 1.78          |
| (2,1794) | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ3  | 4        | 1.78          |
| (2,1794) | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ3  | 4        | 1.78          |
| (2,1145) | 2:205:B:TRP:HE3  | 2:219:B:THR:HA   | 19       | 1.78          |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 10       | 1.77          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD11 | 9        | 1.76          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD12 | 9        | 1.76          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD13 | 9        | 1.76          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 15       | 1.76          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD11 | 6        | 1.75          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD12 | 6        | 1.75          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD13 | 6        | 1.75          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD21 | 6        | 1.75          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD22 | 6        | 1.75          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD23 | 6        | 1.75          |
| (2,2149) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG2  | 14       | 1.75          |
| (2,2149) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG2  | 14       | 1.75          |
| (2,28)   | 1:69:A:GLU:HA    | 2:205:B:TRP:HZ3  | 11       | 1.75          |
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 7        | 1.74          |
| (2,11)   | 2:204:B:THR:HA   | 2:205:B:TRP:HD1  | 19       | 1.74          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 13       | 1.73          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 13       | 1.73          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 13       | 1.73          |
| (2,2149) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG2  | 1        | 1.72          |
| (2,2149) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG2  | 1        | 1.72          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD11 | 4        | 1.72          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD12 | 4        | 1.72          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD13 | 4        | 1.72          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD21 | 4        | 1.72          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD22 | 4        | 1.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD23 | 4        | 1.72          |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H    | 4        | 1.72          |
| (2,1340) | 2:205:B:TRP:HE3  | 2:219:B:THR:H    | 2        | 1.72          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 5        | 1.71          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 5        | 1.71          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 5        | 1.71          |
| (2,1144) | 2:205:B:TRP:HZ3  | 2:219:B:THR:HA   | 1        | 1.71          |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3  | 13       | 1.71          |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3  | 13       | 1.71          |
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3  | 13       | 1.71          |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H    | 13       | 1.7           |
| (2,189)  | 1:70:A:ILE:HG12  | 2:205:B:TRP:HH2  | 20       | 1.7           |
| (2,1145) | 2:205:B:TRP:HE3  | 2:219:B:THR:HA   | 15       | 1.69          |
| (2,531)  | 1:76:A:THR:HG21  | 2:215:B:LYS:HD3  | 17       | 1.69          |
| (2,531)  | 1:76:A:THR:HG22  | 2:215:B:LYS:HD3  | 17       | 1.69          |
| (2,531)  | 1:76:A:THR:HG23  | 2:215:B:LYS:HD3  | 17       | 1.69          |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3  | 15       | 1.69          |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3  | 15       | 1.69          |
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3  | 15       | 1.69          |
| (2,1794) | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ3  | 3        | 1.67          |
| (2,1794) | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ3  | 3        | 1.67          |
| (2,1794) | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ3  | 3        | 1.67          |
| (2,1794) | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ3  | 3        | 1.67          |
| (2,1794) | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ3  | 3        | 1.67          |
| (2,1794) | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ3  | 3        | 1.67          |
| (2,28)   | 1:69:A:GLU:HA    | 2:205:B:TRP:HZ3  | 12       | 1.67          |
| (2,11)   | 2:204:B:THR:HA   | 2:205:B:TRP:HD1  | 3        | 1.67          |
| (2,1407) | 2:213:B:PRO:HG2  | 2:214:B:LEU:H    | 9        | 1.66          |
| (2,15)   | 1:70:A:ILE:HG13  | 2:205:B:TRP:HZ3  | 15       | 1.66          |
| (2,2200) | 2:214:B:LEU:HD11 | 2:215:B:LYS:HG3  | 10       | 1.65          |
| (2,2200) | 2:214:B:LEU:HD12 | 2:215:B:LYS:HG3  | 10       | 1.65          |
| (2,2200) | 2:214:B:LEU:HD13 | 2:215:B:LYS:HG3  | 10       | 1.65          |
| (2,2200) | 2:214:B:LEU:HD21 | 2:215:B:LYS:HG3  | 10       | 1.65          |
| (2,2200) | 2:214:B:LEU:HD22 | 2:215:B:LYS:HG3  | 10       | 1.65          |
| (2,2200) | 2:214:B:LEU:HD23 | 2:215:B:LYS:HG3  | 10       | 1.65          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE2  | 7        | 1.63          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE3  | 7        | 1.63          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 3        | 1.63          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 3        | 1.63          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 3        | 1.63          |
| (2,14)   | 1:70:A:ILE:HD11  | 2:205:B:TRP:HZ3  | 4        | 1.63          |
| (2,14)   | 1:70:A:ILE:HD12  | 2:205:B:TRP:HZ3  | 4        | 1.63          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,14)   | 1:70:A:ILE:HD13  | 2:205:B:TRP:HZ3 | 4        | 1.63          |
| (2,1286) | 1:74:A:PHE:H     | 2:215:B:LYS:HG3 | 11       | 1.62          |
| (2,2127) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HG  | 18       | 1.61          |
| (2,2127) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HG  | 18       | 1.61          |
| (2,2127) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HG  | 18       | 1.61          |
| (2,2127) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HG  | 18       | 1.61          |
| (2,2127) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HG  | 18       | 1.61          |
| (2,2127) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HG  | 18       | 1.61          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H   | 14       | 1.61          |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG  | 15       | 1.61          |
| (2,1251) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HG  | 18       | 1.61          |
| (2,76)   | 1:75:A:GLU:HG3   | 2:214:B:LEU:HB2 | 3        | 1.61          |
| (2,16)   | 2:205:B:TRP:HZ3  | 2:218:B:LEU:HB3 | 8        | 1.61          |
| (2,15)   | 1:70:A:ILE:HG13  | 2:205:B:TRP:HZ3 | 13       | 1.61          |
| (2,11)   | 2:204:B:THR:HA   | 2:205:B:TRP:HD1 | 17       | 1.6           |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD2 | 9        | 1.59          |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD3 | 9        | 1.59          |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD2 | 9        | 1.59          |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD3 | 9        | 1.59          |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H   | 8        | 1.59          |
| (2,2154) | 2:208:B:GLN:HE22 | 2:217:B:ARG:HD2 | 2        | 1.58          |
| (2,2154) | 2:208:B:GLN:HE22 | 2:217:B:ARG:HD3 | 2        | 1.58          |
| (2,1333) | 1:34:A:ARG:HG2   | 2:213:B:PRO:HG3 | 13       | 1.58          |
| (2,1286) | 1:74:A:PHE:H     | 2:215:B:LYS:HG3 | 10       | 1.58          |
| (2,101)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HH2 | 4        | 1.58          |
| (2,101)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HH2 | 4        | 1.58          |
| (2,101)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HH2 | 4        | 1.58          |
| (2,2154) | 2:208:B:GLN:HE22 | 2:217:B:ARG:HD2 | 20       | 1.57          |
| (2,2154) | 2:208:B:GLN:HE22 | 2:217:B:ARG:HD3 | 20       | 1.57          |
| (2,1231) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HA  | 13       | 1.56          |
| (2,1126) | 1:70:A:ILE:H     | 2:205:B:TRP:HE3 | 8        | 1.56          |
| (2,1231) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HA  | 8        | 1.55          |
| (2,2149) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG2 | 15       | 1.54          |
| (2,2149) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG2 | 15       | 1.54          |
| (2,1479) | 2:208:B:GLN:HE21 | 2:219:B:THR:HB  | 14       | 1.54          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H   | 9        | 1.54          |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG  | 10       | 1.54          |
| (2,2150) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG3 | 1        | 1.53          |
| (2,2150) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG3 | 1        | 1.53          |
| (2,1426) | 2:214:B:LEU:H    | 2:215:B:LYS:HG3 | 12       | 1.53          |
| (2,1127) | 1:70:A:ILE:H     | 2:205:B:TRP:HH2 | 20       | 1.53          |
| (2,752)  | 1:75:A:GLU:H     | 2:214:B:LEU:HG  | 13       | 1.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD2  | 2        | 1.52          |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD3  | 2        | 1.52          |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD2  | 2        | 1.52          |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD3  | 2        | 1.52          |
| (2,1340) | 2:205:B:TRP:HE3  | 2:219:B:THR:H    | 12       | 1.52          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD11 | 3        | 1.51          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD12 | 3        | 1.51          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD13 | 3        | 1.51          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 3        | 1.51          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 3        | 1.51          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 3        | 1.51          |
| (2,1334) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HG3  | 3        | 1.51          |
| (2,720)  | 1:74:A:PHE:H     | 2:215:B:LYS:HG2  | 10       | 1.51          |
| (2,1163) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HB3  | 20       | 1.5           |
| (2,1145) | 2:205:B:TRP:HE3  | 2:219:B:THR:HA   | 11       | 1.5           |
| (2,650)  | 1:70:A:ILE:HB    | 2:205:B:TRP:HZ3  | 20       | 1.5           |
| (2,3)    | 2:205:B:TRP:HE3  | 2:218:B:LEU:HB3  | 19       | 1.5           |
| (2,2153) | 2:208:B:GLN:HG2  | 2:219:B:THR:HG21 | 20       | 1.49          |
| (2,2153) | 2:208:B:GLN:HG2  | 2:219:B:THR:HG22 | 20       | 1.49          |
| (2,2153) | 2:208:B:GLN:HG2  | 2:219:B:THR:HG23 | 20       | 1.49          |
| (2,2153) | 2:208:B:GLN:HG3  | 2:219:B:THR:HG21 | 20       | 1.49          |
| (2,2153) | 2:208:B:GLN:HG3  | 2:219:B:THR:HG22 | 20       | 1.49          |
| (2,2153) | 2:208:B:GLN:HG3  | 2:219:B:THR:HG23 | 20       | 1.49          |
| (2,2149) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG2  | 8        | 1.48          |
| (2,2149) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG2  | 8        | 1.48          |
| (2,2150) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG3  | 14       | 1.47          |
| (2,2150) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG3  | 14       | 1.47          |
| (2,1231) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HA   | 15       | 1.47          |
| (2,1931) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG3  | 2        | 1.46          |
| (2,1931) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG3  | 2        | 1.46          |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H    | 5        | 1.46          |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 17       | 1.45          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD11 | 6        | 1.45          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD12 | 6        | 1.45          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD13 | 6        | 1.45          |
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 11       | 1.45          |
| (2,1163) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HB3  | 17       | 1.45          |
| (2,1267) | 2:205:B:TRP:HE3  | 2:220:B:ARG:HB3  | 6        | 1.44          |
| (2,1206) | 1:73:A:ASP:HA    | 2:215:B:LYS:HG3  | 10       | 1.44          |
| (2,189)  | 1:70:A:ILE:HG12  | 2:205:B:TRP:HH2  | 2        | 1.44          |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3  | 7        | 1.44          |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3  | 7        | 1.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3  | 7        | 1.44          |
| (2,1489) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE3  | 2        | 1.43          |
| (2,1334) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HG3  | 15       | 1.43          |
| (2,1231) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HA   | 20       | 1.43          |
| (2,613)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ2  | 3        | 1.43          |
| (2,613)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ2  | 3        | 1.43          |
| (2,613)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ2  | 3        | 1.43          |
| (2,2148) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HB3  | 20       | 1.42          |
| (2,2148) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HB3  | 20       | 1.42          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD11 | 19       | 1.42          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD12 | 19       | 1.42          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD13 | 19       | 1.42          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD21 | 19       | 1.42          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD22 | 19       | 1.42          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD23 | 19       | 1.42          |
| (2,1267) | 2:205:B:TRP:HE3  | 2:220:B:ARG:HB3  | 5        | 1.42          |
| (2,991)  | 1:70:A:ILE:H     | 2:205:B:TRP:HZ3  | 12       | 1.42          |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3  | 9        | 1.42          |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3  | 9        | 1.42          |
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3  | 9        | 1.42          |
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 1        | 1.41          |
| (2,160)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ3  | 4        | 1.41          |
| (2,160)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ3  | 4        | 1.41          |
| (2,160)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ3  | 4        | 1.41          |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD2  | 1        | 1.4           |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD3  | 1        | 1.4           |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD2  | 1        | 1.4           |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD3  | 1        | 1.4           |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3  | 3        | 1.4           |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3  | 3        | 1.4           |
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3  | 3        | 1.4           |
| (2,16)   | 2:205:B:TRP:HZ3  | 2:218:B:LEU:HB3  | 20       | 1.39          |
| (2,2112) | 2:206:B:ARG:HD2  | 2:207:B:VAL:H    | 20       | 1.37          |
| (2,2112) | 2:206:B:ARG:HD3  | 2:207:B:VAL:H    | 20       | 1.37          |
| (2,1206) | 1:73:A:ASP:HA    | 2:215:B:LYS:HG3  | 11       | 1.37          |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3  | 12       | 1.37          |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3  | 12       | 1.37          |
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3  | 12       | 1.37          |
| (2,11)   | 2:204:B:THR:HA   | 2:205:B:TRP:HD1  | 13       | 1.37          |
| (2,2200) | 2:214:B:LEU:HD11 | 2:215:B:LYS:HG3  | 20       | 1.36          |
| (2,2200) | 2:214:B:LEU:HD12 | 2:215:B:LYS:HG3  | 20       | 1.36          |
| (2,2200) | 2:214:B:LEU:HD13 | 2:215:B:LYS:HG3  | 20       | 1.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2200) | 2:214:B:LEU:HD21 | 2:215:B:LYS:HG3  | 20       | 1.36          |
| (2,2200) | 2:214:B:LEU:HD22 | 2:215:B:LYS:HG3  | 20       | 1.36          |
| (2,2200) | 2:214:B:LEU:HD23 | 2:215:B:LYS:HG3  | 20       | 1.36          |
| (2,2110) | 2:206:B:ARG:HG2  | 2:221:B:GLU:H    | 2        | 1.36          |
| (2,2110) | 2:206:B:ARG:HG3  | 2:221:B:GLU:H    | 2        | 1.36          |
| (2,1453) | 2:218:B:LEU:H    | 2:219:B:THR:HG21 | 7        | 1.36          |
| (2,1453) | 2:218:B:LEU:H    | 2:219:B:THR:HG22 | 7        | 1.36          |
| (2,1453) | 2:218:B:LEU:H    | 2:219:B:THR:HG23 | 7        | 1.36          |
| (2,101)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HH2  | 3        | 1.36          |
| (2,101)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HH2  | 3        | 1.36          |
| (2,101)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HH2  | 3        | 1.36          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE2  | 20       | 1.35          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE3  | 20       | 1.35          |
| (2,2109) | 2:206:B:ARG:HG2  | 2:220:B:ARG:HA   | 2        | 1.35          |
| (2,2109) | 2:206:B:ARG:HG3  | 2:220:B:ARG:HA   | 2        | 1.35          |
| (2,1475) | 1:73:A:ASP:HA    | 2:216:B:ILE:H    | 13       | 1.35          |
| (2,2092) | 2:205:B:TRP:HB3  | 2:220:B:ARG:HD2  | 12       | 1.34          |
| (2,2092) | 2:205:B:TRP:HB3  | 2:220:B:ARG:HD3  | 12       | 1.34          |
| (2,1486) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB3  | 9        | 1.34          |
| (2,1398) | 1:68:A:ASP:HB2   | 2:220:B:ARG:H    | 1        | 1.34          |
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 14       | 1.34          |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H    | 1        | 1.33          |
| (2,1333) | 1:34:A:ARG:HG2   | 2:213:B:PRO:HG3  | 6        | 1.32          |
| (2,720)  | 1:74:A:PHE:H     | 2:215:B:LYS:HG2  | 12       | 1.32          |
| (2,1484) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HG3  | 10       | 1.31          |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3  | 18       | 1.31          |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3  | 18       | 1.31          |
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3  | 18       | 1.31          |
| (2,16)   | 2:205:B:TRP:HZ3  | 2:218:B:LEU:HB3  | 13       | 1.3           |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB2  | 13       | 1.29          |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB3  | 13       | 1.29          |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB2  | 17       | 1.29          |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB3  | 17       | 1.29          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H    | 13       | 1.28          |
| (2,143)  | 1:70:A:ILE:HG13  | 2:205:B:TRP:HH2  | 20       | 1.28          |
| (2,2170) | 2:210:B:SER:HB2  | 2:215:B:LYS:H    | 2        | 1.27          |
| (2,2170) | 2:210:B:SER:HB3  | 2:215:B:LYS:H    | 2        | 1.27          |
| (2,1250) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HG   | 14       | 1.27          |
| (2,1250) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HG   | 14       | 1.27          |
| (2,1224) | 1:70:A:ILE:HD11  | 2:219:B:THR:HA   | 14       | 1.27          |
| (2,1224) | 1:70:A:ILE:HD12  | 2:219:B:THR:HA   | 14       | 1.27          |
| (2,1224) | 1:70:A:ILE:HD13  | 2:219:B:THR:HA   | 14       | 1.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,162)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ3  | 13       | 1.27          |
| (2,162)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ3  | 13       | 1.27          |
| (2,162)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ3  | 13       | 1.27          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 20       | 1.27          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD11 | 13       | 1.26          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD12 | 13       | 1.26          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD13 | 13       | 1.26          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD21 | 13       | 1.26          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD22 | 13       | 1.26          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD23 | 13       | 1.26          |
| (2,1479) | 2:208:B:GLN:HE21 | 2:219:B:THR:HB   | 20       | 1.26          |
| (2,1209) | 1:73:A:ASP:HA    | 2:215:B:LYS:HD2  | 17       | 1.26          |
| (2,160)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ3  | 3        | 1.26          |
| (2,160)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ3  | 3        | 1.26          |
| (2,160)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ3  | 3        | 1.26          |
| (2,76)   | 1:75:A:GLU:HG3   | 2:214:B:LEU:HB2  | 14       | 1.26          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD11 | 6        | 1.25          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD12 | 6        | 1.25          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD13 | 6        | 1.25          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 6        | 1.25          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 6        | 1.25          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 6        | 1.25          |
| (2,2148) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HB3  | 9        | 1.25          |
| (2,2148) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HB3  | 9        | 1.25          |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H    | 19       | 1.25          |
| (2,1225) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HA   | 13       | 1.25          |
| (2,1145) | 2:205:B:TRP:HE3  | 2:219:B:THR:HA   | 2        | 1.25          |
| (2,990)  | 1:69:A:GLU:H     | 2:205:B:TRP:HZ3  | 2        | 1.25          |
| (2,2111) | 2:206:B:ARG:HG2  | 2:221:B:GLU:HG2  | 2        | 1.24          |
| (2,2111) | 2:206:B:ARG:HG2  | 2:221:B:GLU:HG3  | 2        | 1.24          |
| (2,2111) | 2:206:B:ARG:HG3  | 2:221:B:GLU:HG2  | 2        | 1.24          |
| (2,2111) | 2:206:B:ARG:HG3  | 2:221:B:GLU:HG3  | 2        | 1.24          |
| (2,1931) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG3  | 11       | 1.24          |
| (2,1931) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG3  | 11       | 1.24          |
| (2,1931) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG3  | 14       | 1.24          |
| (2,1931) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG3  | 14       | 1.24          |
| (2,1931) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG3  | 20       | 1.24          |
| (2,1931) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG3  | 20       | 1.24          |
| (2,143)  | 1:70:A:ILE:HG13  | 2:205:B:TRP:HH2  | 15       | 1.24          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE2  | 11       | 1.23          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE3  | 11       | 1.23          |
| (2,13)   | 1:70:A:ILE:HG12  | 2:205:B:TRP:HZ3  | 20       | 1.23          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,2187) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE2 | 2        | 1.22          |
| (2,2187) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE3 | 2        | 1.22          |
| (2,1606) | 1:34:A:ARG:HD2   | 2:213:B:PRO:HG3 | 3        | 1.22          |
| (2,1606) | 1:34:A:ARG:HD3   | 2:213:B:PRO:HG3 | 3        | 1.22          |
| (2,1418) | 2:214:B:LEU:H    | 2:215:B:LYS:HB2 | 10       | 1.22          |
| (2,1286) | 1:74:A:PHE:H     | 2:215:B:LYS:HG3 | 2        | 1.22          |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD2 | 12       | 1.21          |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD3 | 12       | 1.21          |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD2 | 12       | 1.21          |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD3 | 12       | 1.21          |
| (2,1231) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HA  | 11       | 1.21          |
| (2,162)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ3 | 15       | 1.21          |
| (2,162)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ3 | 15       | 1.21          |
| (2,162)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ3 | 15       | 1.21          |
| (2,1484) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HG3 | 12       | 1.2           |
| (2,1212) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HD2 | 9        | 1.2           |
| (2,1176) | 2:210:B:SER:HB2  | 2:215:B:LYS:HB3 | 6        | 1.2           |
| (2,613)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ2 | 4        | 1.2           |
| (2,613)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ2 | 4        | 1.2           |
| (2,613)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ2 | 4        | 1.2           |
| (2,2148) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HB3 | 2        | 1.19          |
| (2,2148) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HB3 | 2        | 1.19          |
| (2,2109) | 2:206:B:ARG:HG2  | 2:220:B:ARG:HA  | 8        | 1.19          |
| (2,2109) | 2:206:B:ARG:HG3  | 2:220:B:ARG:HA  | 8        | 1.19          |
| (2,1606) | 1:34:A:ARG:HD2   | 2:213:B:PRO:HG3 | 9        | 1.19          |
| (2,1606) | 1:34:A:ARG:HD3   | 2:213:B:PRO:HG3 | 9        | 1.19          |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H   | 3        | 1.19          |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H   | 6        | 1.19          |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB2 | 6        | 1.18          |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB3 | 6        | 1.18          |
| (2,1209) | 1:73:A:ASP:HA    | 2:215:B:LYS:HD2 | 18       | 1.18          |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG  | 5        | 1.17          |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG  | 13       | 1.17          |
| (2,1286) | 1:74:A:PHE:H     | 2:215:B:LYS:HG3 | 20       | 1.17          |
| (2,76)   | 1:75:A:GLU:HG3   | 2:214:B:LEU:HB2 | 15       | 1.17          |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3 | 17       | 1.17          |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3 | 17       | 1.17          |
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3 | 17       | 1.17          |
| (2,1333) | 1:34:A:ARG:HG2   | 2:213:B:PRO:HG3 | 9        | 1.16          |
| (2,615)  | 1:75:A:GLU:HG2   | 2:214:B:LEU:HB2 | 3        | 1.16          |
| (2,2172) | 2:210:B:SER:HB2  | 2:215:B:LYS:HD2 | 9        | 1.15          |
| (2,2172) | 2:210:B:SER:HB3  | 2:215:B:LYS:HD2 | 9        | 1.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1931) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG3  | 9        | 1.15          |
| (2,1931) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG3  | 9        | 1.15          |
| (2,1176) | 2:210:B:SER:HB2  | 2:215:B:LYS:HB3  | 2        | 1.15          |
| (2,650)  | 1:70:A:ILE:HB    | 2:205:B:TRP:HZ3  | 11       | 1.15          |
| (2,613)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ2  | 18       | 1.15          |
| (2,613)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ2  | 18       | 1.15          |
| (2,613)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ2  | 18       | 1.15          |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD2  | 14       | 1.14          |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD3  | 14       | 1.14          |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD2  | 14       | 1.14          |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD3  | 14       | 1.14          |
| (2,2150) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG3  | 8        | 1.14          |
| (2,2150) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG3  | 8        | 1.14          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD11 | 13       | 1.14          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD12 | 13       | 1.14          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD13 | 13       | 1.14          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD21 | 13       | 1.14          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD22 | 13       | 1.14          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD23 | 13       | 1.14          |
| (2,1606) | 1:34:A:ARG:HD2   | 2:213:B:PRO:HG3  | 15       | 1.14          |
| (2,1606) | 1:34:A:ARG:HD3   | 2:213:B:PRO:HG3  | 15       | 1.14          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H    | 20       | 1.14          |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3  | 8        | 1.14          |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3  | 8        | 1.14          |
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3  | 8        | 1.14          |
| (2,2112) | 2:206:B:ARG:HD2  | 2:207:B:VAL:H    | 1        | 1.13          |
| (2,2112) | 2:206:B:ARG:HD3  | 2:207:B:VAL:H    | 1        | 1.13          |
| (2,2084) | 2:205:B:TRP:H    | 2:220:B:ARG:HG2  | 10       | 1.13          |
| (2,2084) | 2:205:B:TRP:H    | 2:220:B:ARG:HG3  | 10       | 1.13          |
| (2,1177) | 2:210:B:SER:HB2  | 2:215:B:LYS:HB2  | 6        | 1.13          |
| (2,16)   | 2:205:B:TRP:HZ3  | 2:218:B:LEU:HB3  | 11       | 1.13          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE2  | 10       | 1.12          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE3  | 10       | 1.12          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD11 | 17       | 1.12          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD12 | 17       | 1.12          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD13 | 17       | 1.12          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD21 | 17       | 1.12          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD22 | 17       | 1.12          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD23 | 17       | 1.12          |
| (2,1479) | 2:208:B:GLN:HE21 | 2:219:B:THR:HB   | 2        | 1.12          |
| (2,1391) | 2:209:B:ARG:HD2  | 2:210:B:SER:H    | 4        | 1.12          |
| (2,2165) | 2:209:B:ARG:HD2  | 2:210:B:SER:H    | 4        | 1.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2165) | 2:209:B:ARG:HD3  | 2:210:B:SER:H    | 4        | 1.11          |
| (2,1479) | 2:208:B:GLN:HE21 | 2:219:B:THR:HB   | 8        | 1.11          |
| (2,1204) | 1:73:A:ASP:HA    | 2:215:B:LYS:HG2  | 10       | 1.11          |
| (2,76)   | 1:75:A:GLU:HG3   | 2:214:B:LEU:HB2  | 13       | 1.11          |
| (2,2153) | 2:208:B:GLN:HG2  | 2:219:B:THR:HG21 | 7        | 1.1           |
| (2,2153) | 2:208:B:GLN:HG2  | 2:219:B:THR:HG22 | 7        | 1.1           |
| (2,2153) | 2:208:B:GLN:HG2  | 2:219:B:THR:HG23 | 7        | 1.1           |
| (2,2153) | 2:208:B:GLN:HG3  | 2:219:B:THR:HG21 | 7        | 1.1           |
| (2,2153) | 2:208:B:GLN:HG3  | 2:219:B:THR:HG22 | 7        | 1.1           |
| (2,2153) | 2:208:B:GLN:HG3  | 2:219:B:THR:HG23 | 7        | 1.1           |
| (2,1794) | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ3  | 18       | 1.1           |
| (2,1794) | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ3  | 18       | 1.1           |
| (2,1794) | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ3  | 18       | 1.1           |
| (2,1794) | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ3  | 18       | 1.1           |
| (2,1794) | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ3  | 18       | 1.1           |
| (2,1794) | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ3  | 18       | 1.1           |
| (2,1479) | 2:208:B:GLN:HE21 | 2:219:B:THR:HB   | 3        | 1.1           |
| (2,1145) | 2:205:B:TRP:HE3  | 2:219:B:THR:HA   | 20       | 1.1           |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG21 | 9        | 1.1           |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG22 | 9        | 1.1           |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG23 | 9        | 1.1           |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD11 | 15       | 1.09          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD12 | 15       | 1.09          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD13 | 15       | 1.09          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD21 | 15       | 1.09          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD22 | 15       | 1.09          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD23 | 15       | 1.09          |
| (2,1931) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG3  | 13       | 1.09          |
| (2,1931) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG3  | 13       | 1.09          |
| (2,1908) | 1:69:A:GLU:HG2   | 2:217:B:ARG:HD2  | 11       | 1.09          |
| (2,1908) | 1:69:A:GLU:HG2   | 2:217:B:ARG:HD3  | 11       | 1.09          |
| (2,1908) | 1:69:A:GLU:HG3   | 2:217:B:ARG:HD2  | 11       | 1.09          |
| (2,1908) | 1:69:A:GLU:HG3   | 2:217:B:ARG:HD3  | 11       | 1.09          |
| (2,1392) | 2:209:B:ARG:HD3  | 2:210:B:SER:H    | 4        | 1.09          |
| (2,1237) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB2  | 10       | 1.09          |
| (2,1178) | 2:210:B:SER:HB3  | 2:215:B:LYS:HB2  | 2        | 1.09          |
| (2,1163) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HB3  | 13       | 1.09          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H    | 15       | 1.08          |
| (2,1277) | 1:71:A:GLU:HG2   | 2:217:B:ARG:HG3  | 8        | 1.08          |
| (2,100)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HH2  | 13       | 1.08          |
| (2,100)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HH2  | 13       | 1.08          |
| (2,100)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HH2  | 13       | 1.08          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 18       | 1.08          |
| (2,1367) | 1:73:A:ASP:HA    | 2:215:B:LYS:H    | 13       | 1.07          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 10       | 1.07          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 10       | 1.07          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 10       | 1.07          |
| (2,2109) | 2:206:B:ARG:HG2  | 2:220:B:ARG:HA   | 11       | 1.06          |
| (2,2109) | 2:206:B:ARG:HG3  | 2:220:B:ARG:HA   | 11       | 1.06          |
| (2,1486) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB3  | 17       | 1.06          |
| (2,1206) | 1:73:A:ASP:HA    | 2:215:B:LYS:HG3  | 20       | 1.06          |
| (2,2177) | 2:212:B:ASN:H    | 2:215:B:LYS:HE2  | 20       | 1.05          |
| (2,2177) | 2:212:B:ASN:H    | 2:215:B:LYS:HE3  | 20       | 1.05          |
| (2,2150) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG3  | 15       | 1.05          |
| (2,2150) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG3  | 15       | 1.05          |
| (2,1355) | 1:74:A:PHE:HD1   | 2:214:B:LEU:H    | 14       | 1.05          |
| (2,1355) | 1:74:A:PHE:HD2   | 2:214:B:LEU:H    | 14       | 1.05          |
| (2,208)  | 1:69:A:GLU:HA    | 2:205:B:TRP:HE3  | 20       | 1.05          |
| (2,1489) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE3  | 20       | 1.04          |
| (2,1383) | 2:206:B:ARG:H    | 2:220:B:ARG:HA   | 8        | 1.04          |
| (2,1272) | 1:69:A:GLU:HG2   | 2:219:B:THR:HB   | 8        | 1.04          |
| (2,23)   | 1:70:A:ILE:HD11  | 2:205:B:TRP:HH2  | 8        | 1.04          |
| (2,23)   | 1:70:A:ILE:HD12  | 2:205:B:TRP:HH2  | 8        | 1.04          |
| (2,23)   | 1:70:A:ILE:HD13  | 2:205:B:TRP:HH2  | 8        | 1.04          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD11 | 15       | 1.03          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD12 | 15       | 1.03          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD13 | 15       | 1.03          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD21 | 15       | 1.03          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD22 | 15       | 1.03          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD23 | 15       | 1.03          |
| (2,1910) | 1:69:A:GLU:HG2   | 2:219:B:THR:HG21 | 1        | 1.03          |
| (2,1910) | 1:69:A:GLU:HG2   | 2:219:B:THR:HG22 | 1        | 1.03          |
| (2,1910) | 1:69:A:GLU:HG2   | 2:219:B:THR:HG23 | 1        | 1.03          |
| (2,1910) | 1:69:A:GLU:HG3   | 2:219:B:THR:HG21 | 1        | 1.03          |
| (2,1910) | 1:69:A:GLU:HG3   | 2:219:B:THR:HG22 | 1        | 1.03          |
| (2,1910) | 1:69:A:GLU:HG3   | 2:219:B:THR:HG23 | 1        | 1.03          |
| (2,1475) | 1:73:A:ASP:HA    | 2:216:B:ILE:H    | 15       | 1.03          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD11 | 3        | 1.03          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD12 | 3        | 1.03          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD13 | 3        | 1.03          |
| (2,1209) | 1:73:A:ASP:HA    | 2:215:B:LYS:HD2  | 12       | 1.03          |
| (2,1144) | 2:205:B:TRP:HZ3  | 2:219:B:THR:HA   | 9        | 1.03          |
| (2,720)  | 1:74:A:PHE:H     | 2:215:B:LYS:HG2  | 2        | 1.03          |
| (2,16)   | 2:205:B:TRP:HZ3  | 2:218:B:LEU:HB3  | 15       | 1.03          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2149) | 2:208:B:GLN:HG2 | 2:217:B:ARG:HG2  | 18       | 1.02          |
| (2,2149) | 2:208:B:GLN:HG3 | 2:217:B:ARG:HG2  | 18       | 1.02          |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD11 | 17       | 1.02          |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD12 | 17       | 1.02          |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD13 | 17       | 1.02          |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD21 | 17       | 1.02          |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD22 | 17       | 1.02          |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD23 | 17       | 1.02          |
| (2,1267) | 2:205:B:TRP:HE3 | 2:220:B:ARG:HB3  | 1        | 1.02          |
| (2,1206) | 1:73:A:ASP:HA   | 2:215:B:LYS:HG3  | 2        | 1.02          |
| (2,58)   | 1:76:A:THR:HG21 | 2:215:B:LYS:HG3  | 19       | 1.02          |
| (2,58)   | 1:76:A:THR:HG22 | 2:215:B:LYS:HG3  | 19       | 1.02          |
| (2,58)   | 1:76:A:THR:HG23 | 2:215:B:LYS:HG3  | 19       | 1.02          |
| (2,2109) | 2:206:B:ARG:HG2 | 2:220:B:ARG:HA   | 14       | 1.01          |
| (2,2109) | 2:206:B:ARG:HG3 | 2:220:B:ARG:HA   | 14       | 1.01          |
| (2,2096) | 2:205:B:TRP:HZ2 | 2:218:B:LEU:HD11 | 3        | 1.01          |
| (2,2096) | 2:205:B:TRP:HZ2 | 2:218:B:LEU:HD12 | 3        | 1.01          |
| (2,2096) | 2:205:B:TRP:HZ2 | 2:218:B:LEU:HD13 | 3        | 1.01          |
| (2,2096) | 2:205:B:TRP:HZ2 | 2:218:B:LEU:HD21 | 3        | 1.01          |
| (2,2096) | 2:205:B:TRP:HZ2 | 2:218:B:LEU:HD22 | 3        | 1.01          |
| (2,2096) | 2:205:B:TRP:HZ2 | 2:218:B:LEU:HD23 | 3        | 1.01          |
| (2,1606) | 1:34:A:ARG:HD2  | 2:213:B:PRO:HG3  | 5        | 1.01          |
| (2,1606) | 1:34:A:ARG:HD3  | 2:213:B:PRO:HG3  | 5        | 1.01          |
| (2,1224) | 1:70:A:ILE:HD11 | 2:219:B:THR:HA   | 9        | 1.01          |
| (2,1224) | 1:70:A:ILE:HD12 | 2:219:B:THR:HA   | 9        | 1.01          |
| (2,1224) | 1:70:A:ILE:HD13 | 2:219:B:THR:HA   | 9        | 1.01          |
| (2,1137) | 1:70:A:ILE:H    | 2:219:B:THR:HG21 | 14       | 1.01          |
| (2,1137) | 1:70:A:ILE:H    | 2:219:B:THR:HG22 | 14       | 1.01          |
| (2,1137) | 1:70:A:ILE:H    | 2:219:B:THR:HG23 | 14       | 1.01          |
| (2,2151) | 2:208:B:GLN:HG2 | 2:217:B:ARG:HD2  | 8        | 1.0           |
| (2,2151) | 2:208:B:GLN:HG2 | 2:217:B:ARG:HD3  | 8        | 1.0           |
| (2,2151) | 2:208:B:GLN:HG3 | 2:217:B:ARG:HD2  | 8        | 1.0           |
| (2,2151) | 2:208:B:GLN:HG3 | 2:217:B:ARG:HD3  | 8        | 1.0           |
| (2,1474) | 1:75:A:GLU:HG2  | 2:215:B:LYS:H    | 6        | 1.0           |
| (2,1127) | 1:70:A:ILE:H    | 2:205:B:TRP:HH2  | 2        | 1.0           |
| (2,1910) | 1:69:A:GLU:HG2  | 2:219:B:THR:HG21 | 9        | 0.99          |
| (2,1910) | 1:69:A:GLU:HG2  | 2:219:B:THR:HG22 | 9        | 0.99          |
| (2,1910) | 1:69:A:GLU:HG2  | 2:219:B:THR:HG23 | 9        | 0.99          |
| (2,1910) | 1:69:A:GLU:HG3  | 2:219:B:THR:HG21 | 9        | 0.99          |
| (2,1910) | 1:69:A:GLU:HG3  | 2:219:B:THR:HG22 | 9        | 0.99          |
| (2,1910) | 1:69:A:GLU:HG3  | 2:219:B:THR:HG23 | 9        | 0.99          |
| (2,1794) | 1:52:A:VAL:HG11 | 2:205:B:TRP:HZ3  | 8        | 0.99          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1794) | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ3  | 8        | 0.99          |
| (2,1794) | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ3  | 8        | 0.99          |
| (2,1794) | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ3  | 8        | 0.99          |
| (2,1794) | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ3  | 8        | 0.99          |
| (2,1794) | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ3  | 8        | 0.99          |
| (2,1214) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD11 | 13       | 0.99          |
| (2,1214) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD12 | 13       | 0.99          |
| (2,1214) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD13 | 13       | 0.99          |
| (2,1163) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HB3  | 12       | 0.99          |
| (2,1930) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG2  | 12       | 0.98          |
| (2,1930) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG2  | 12       | 0.98          |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB2  | 9        | 0.98          |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB3  | 9        | 0.98          |
| (2,1407) | 2:213:B:PRO:HG2  | 2:214:B:LEU:H    | 6        | 0.98          |
| (2,1126) | 1:70:A:ILE:H     | 2:205:B:TRP:HE3  | 13       | 0.98          |
| (2,189)  | 1:70:A:ILE:HG12  | 2:205:B:TRP:HH2  | 6        | 0.98          |
| (2,28)   | 1:69:A:GLU:HA    | 2:205:B:TRP:HZ3  | 5        | 0.98          |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG   | 18       | 0.97          |
| (2,1929) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HA   | 13       | 0.96          |
| (2,1929) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HA   | 13       | 0.96          |
| (2,1398) | 1:68:A:ASP:HB2   | 2:220:B:ARG:H    | 9        | 0.96          |
| (2,1163) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HB3  | 11       | 0.96          |
| (2,2149) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG2  | 3        | 0.95          |
| (2,2149) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG2  | 3        | 0.95          |
| (2,1606) | 1:34:A:ARG:HD2   | 2:213:B:PRO:HG3  | 18       | 0.95          |
| (2,1606) | 1:34:A:ARG:HD3   | 2:213:B:PRO:HG3  | 18       | 0.95          |
| (2,1488) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HD3  | 9        | 0.95          |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H    | 17       | 0.95          |
| (2,1334) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HG3  | 5        | 0.95          |
| (2,1294) | 2:204:B:THR:HG21 | 2:205:B:TRP:HD1  | 17       | 0.95          |
| (2,1294) | 2:204:B:THR:HG22 | 2:205:B:TRP:HD1  | 17       | 0.95          |
| (2,1294) | 2:204:B:THR:HG23 | 2:205:B:TRP:HD1  | 17       | 0.95          |
| (2,1214) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD11 | 15       | 0.95          |
| (2,1214) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD12 | 15       | 0.95          |
| (2,1214) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD13 | 15       | 0.95          |
| (2,2207) | 2:216:B:ILE:HG13 | 2:218:B:LEU:HD11 | 18       | 0.94          |
| (2,2207) | 2:216:B:ILE:HG13 | 2:218:B:LEU:HD12 | 18       | 0.94          |
| (2,2207) | 2:216:B:ILE:HG13 | 2:218:B:LEU:HD13 | 18       | 0.94          |
| (2,2207) | 2:216:B:ILE:HG13 | 2:218:B:LEU:HD21 | 18       | 0.94          |
| (2,2207) | 2:216:B:ILE:HG13 | 2:218:B:LEU:HD22 | 18       | 0.94          |
| (2,2207) | 2:216:B:ILE:HG13 | 2:218:B:LEU:HD23 | 18       | 0.94          |
| (2,2191) | 2:213:B:PRO:HB2  | 2:214:B:LEU:HD11 | 9        | 0.94          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2191) | 2:213:B:PRO:HB2  | 2:214:B:LEU:HD12 | 9        | 0.94          |
| (2,2191) | 2:213:B:PRO:HB2  | 2:214:B:LEU:HD13 | 9        | 0.94          |
| (2,2191) | 2:213:B:PRO:HB2  | 2:214:B:LEU:HD21 | 9        | 0.94          |
| (2,2191) | 2:213:B:PRO:HB2  | 2:214:B:LEU:HD22 | 9        | 0.94          |
| (2,2191) | 2:213:B:PRO:HB2  | 2:214:B:LEU:HD23 | 9        | 0.94          |
| (2,2191) | 2:213:B:PRO:HB3  | 2:214:B:LEU:HD11 | 9        | 0.94          |
| (2,2191) | 2:213:B:PRO:HB3  | 2:214:B:LEU:HD12 | 9        | 0.94          |
| (2,2191) | 2:213:B:PRO:HB3  | 2:214:B:LEU:HD13 | 9        | 0.94          |
| (2,2191) | 2:213:B:PRO:HB3  | 2:214:B:LEU:HD21 | 9        | 0.94          |
| (2,2191) | 2:213:B:PRO:HB3  | 2:214:B:LEU:HD22 | 9        | 0.94          |
| (2,2191) | 2:213:B:PRO:HB3  | 2:214:B:LEU:HD23 | 9        | 0.94          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD11 | 3        | 0.94          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD12 | 3        | 0.94          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD13 | 3        | 0.94          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD21 | 3        | 0.94          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD22 | 3        | 0.94          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD23 | 3        | 0.94          |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 9        | 0.94          |
| (2,1479) | 2:208:B:GLN:HE21 | 2:219:B:THR:HB   | 1        | 0.94          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H    | 3        | 0.94          |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG   | 3        | 0.94          |
| (2,1334) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HG3  | 18       | 0.94          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 20       | 0.94          |
| (1,13)   | 1:51:A:VAL:O     | 1:55:A:ILE:N     | 16       | 0.94          |
| (2,2200) | 2:214:B:LEU:HD11 | 2:215:B:LYS:HG3  | 2        | 0.93          |
| (2,2200) | 2:214:B:LEU:HD12 | 2:215:B:LYS:HG3  | 2        | 0.93          |
| (2,2200) | 2:214:B:LEU:HD13 | 2:215:B:LYS:HG3  | 2        | 0.93          |
| (2,2200) | 2:214:B:LEU:HD21 | 2:215:B:LYS:HG3  | 2        | 0.93          |
| (2,2200) | 2:214:B:LEU:HD22 | 2:215:B:LYS:HG3  | 2        | 0.93          |
| (2,2200) | 2:214:B:LEU:HD23 | 2:215:B:LYS:HG3  | 2        | 0.93          |
| (2,2170) | 2:210:B:SER:HB2  | 2:215:B:LYS:H    | 6        | 0.93          |
| (2,2170) | 2:210:B:SER:HB3  | 2:215:B:LYS:H    | 6        | 0.93          |
| (2,1930) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG2  | 2        | 0.93          |
| (2,1930) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG2  | 2        | 0.93          |
| (2,1490) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE2  | 2        | 0.93          |
| (2,1488) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HD3  | 17       | 0.93          |
| (2,1427) | 2:215:B:LYS:H    | 2:215:B:LYS:HG3  | 12       | 0.93          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 8        | 0.93          |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG21 | 1        | 0.93          |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG22 | 1        | 0.93          |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG23 | 1        | 0.93          |
| (2,13)   | 1:70:A:ILE:HG12  | 2:205:B:TRP:HZ3  | 11       | 0.93          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,11)   | 2:204:B:THR:HA   | 2:205:B:TRP:HD1  | 15       | 0.93          |
| (2,1737) | 1:48:A:LEU:HD11  | 2:205:B:TRP:HZ2  | 18       | 0.92          |
| (2,1737) | 1:48:A:LEU:HD12  | 2:205:B:TRP:HZ2  | 18       | 0.92          |
| (2,1737) | 1:48:A:LEU:HD13  | 2:205:B:TRP:HZ2  | 18       | 0.92          |
| (2,1737) | 1:48:A:LEU:HD21  | 2:205:B:TRP:HZ2  | 18       | 0.92          |
| (2,1737) | 1:48:A:LEU:HD22  | 2:205:B:TRP:HZ2  | 18       | 0.92          |
| (2,1737) | 1:48:A:LEU:HD23  | 2:205:B:TRP:HZ2  | 18       | 0.92          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 3        | 0.92          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 18       | 0.92          |
| (2,2170) | 2:210:B:SER:HB2  | 2:215:B:LYS:H    | 4        | 0.91          |
| (2,2170) | 2:210:B:SER:HB3  | 2:215:B:LYS:H    | 4        | 0.91          |
| (2,1489) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE3  | 11       | 0.91          |
| (2,1488) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HD3  | 12       | 0.91          |
| (2,1479) | 2:208:B:GLN:HE21 | 2:219:B:THR:HB   | 18       | 0.91          |
| (2,990)  | 1:69:A:GLU:H     | 2:205:B:TRP:HZ3  | 6        | 0.91          |
| (2,636)  | 1:69:A:GLU:HA    | 2:219:B:THR:HG21 | 9        | 0.91          |
| (2,636)  | 1:69:A:GLU:HA    | 2:219:B:THR:HG22 | 9        | 0.91          |
| (2,636)  | 1:69:A:GLU:HA    | 2:219:B:THR:HG23 | 9        | 0.91          |
| (2,143)  | 1:70:A:ILE:HG13  | 2:205:B:TRP:HH2  | 2        | 0.91          |
| (2,100)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HH2  | 15       | 0.91          |
| (2,100)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HH2  | 15       | 0.91          |
| (2,100)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HH2  | 15       | 0.91          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 16       | 0.91          |
| (2,1930) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG2  | 10       | 0.9           |
| (2,1930) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG2  | 10       | 0.9           |
| (2,1249) | 1:75:A:GLU:H     | 2:214:B:LEU:HD11 | 13       | 0.9           |
| (2,1249) | 1:75:A:GLU:H     | 2:214:B:LEU:HD12 | 13       | 0.9           |
| (2,1249) | 1:75:A:GLU:H     | 2:214:B:LEU:HD13 | 13       | 0.9           |
| (2,1178) | 2:210:B:SER:HB3  | 2:215:B:LYS:HB2  | 4        | 0.9           |
| (2,1126) | 1:70:A:ILE:H     | 2:205:B:TRP:HE3  | 18       | 0.9           |
| (2,752)  | 1:75:A:GLU:H     | 2:214:B:LEU:HG   | 14       | 0.9           |
| (2,1486) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB3  | 1        | 0.89          |
| (2,1479) | 2:208:B:GLN:HE21 | 2:219:B:THR:HB   | 12       | 0.89          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 2        | 0.89          |
| (2,1144) | 2:205:B:TRP:HZ3  | 2:219:B:THR:HA   | 16       | 0.89          |
| (2,1127) | 1:70:A:ILE:H     | 2:205:B:TRP:HH2  | 15       | 0.89          |
| (2,613)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ2  | 8        | 0.89          |
| (2,613)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ2  | 8        | 0.89          |
| (2,613)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ2  | 8        | 0.89          |
| (2,531)  | 1:76:A:THR:HG21  | 2:215:B:LYS:HD3  | 20       | 0.89          |
| (2,531)  | 1:76:A:THR:HG22  | 2:215:B:LYS:HD3  | 20       | 0.89          |
| (2,531)  | 1:76:A:THR:HG23  | 2:215:B:LYS:HD3  | 20       | 0.89          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,208)  | 1:69:A:GLU:HA    | 2:205:B:TRP:HE3  | 15       | 0.89          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE2  | 2        | 0.88          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE3  | 2        | 0.88          |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD11 | 15       | 0.88          |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD12 | 15       | 0.88          |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD13 | 15       | 0.88          |
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 15       | 0.87          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 13       | 0.87          |
| (2,1224) | 1:70:A:ILE:HD11  | 2:219:B:THR:HA   | 1        | 0.87          |
| (2,1224) | 1:70:A:ILE:HD12  | 2:219:B:THR:HA   | 1        | 0.87          |
| (2,1224) | 1:70:A:ILE:HD13  | 2:219:B:THR:HA   | 1        | 0.87          |
| (2,990)  | 1:69:A:GLU:H     | 2:205:B:TRP:HZ3  | 20       | 0.87          |
| (2,803)  | 1:75:A:GLU:H     | 2:214:B:LEU:HB2  | 13       | 0.87          |
| (2,100)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HH2  | 20       | 0.87          |
| (2,100)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HH2  | 20       | 0.87          |
| (2,100)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HH2  | 20       | 0.87          |
| (2,2140) | 2:208:B:GLN:HB2  | 2:217:B:ARG:HD2  | 6        | 0.86          |
| (2,2140) | 2:208:B:GLN:HB2  | 2:217:B:ARG:HD3  | 6        | 0.86          |
| (2,2140) | 2:208:B:GLN:HB3  | 2:217:B:ARG:HD2  | 6        | 0.86          |
| (2,2140) | 2:208:B:GLN:HB3  | 2:217:B:ARG:HD3  | 6        | 0.86          |
| (2,1225) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HA   | 14       | 0.86          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 4        | 0.86          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 4        | 0.86          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 4        | 0.86          |
| (2,1174) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HB2  | 7        | 0.86          |
| (2,1126) | 1:70:A:ILE:H     | 2:205:B:TRP:HE3  | 19       | 0.86          |
| (2,14)   | 1:70:A:ILE:HD11  | 2:205:B:TRP:HZ3  | 15       | 0.86          |
| (2,14)   | 1:70:A:ILE:HD12  | 2:205:B:TRP:HZ3  | 15       | 0.86          |
| (2,14)   | 1:70:A:ILE:HD13  | 2:205:B:TRP:HZ3  | 15       | 0.86          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE2  | 3        | 0.85          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE3  | 3        | 0.85          |
| (2,2148) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HB3  | 1        | 0.85          |
| (2,2148) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HB3  | 1        | 0.85          |
| (2,2141) | 2:208:B:GLN:HB2  | 2:219:B:THR:H    | 5        | 0.85          |
| (2,2141) | 2:208:B:GLN:HB3  | 2:219:B:THR:H    | 5        | 0.85          |
| (2,2112) | 2:206:B:ARG:HD2  | 2:207:B:VAL:H    | 2        | 0.85          |
| (2,2112) | 2:206:B:ARG:HD3  | 2:207:B:VAL:H    | 2        | 0.85          |
| (2,1932) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HD3  | 2        | 0.85          |
| (2,1932) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HD3  | 2        | 0.85          |
| (2,1909) | 1:69:A:GLU:HG2   | 2:219:B:THR:HB   | 9        | 0.85          |
| (2,1909) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 9        | 0.85          |
| (2,1245) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HG3  | 12       | 0.85          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1227) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HA   | 15       | 0.85          |
| (2,1215) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD21 | 14       | 0.85          |
| (2,1215) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD22 | 14       | 0.85          |
| (2,1215) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD23 | 14       | 0.85          |
| (2,531)  | 1:76:A:THR:HG21  | 2:215:B:LYS:HD3  | 1        | 0.85          |
| (2,531)  | 1:76:A:THR:HG22  | 2:215:B:LYS:HD3  | 1        | 0.85          |
| (2,531)  | 1:76:A:THR:HG23  | 2:215:B:LYS:HD3  | 1        | 0.85          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 2        | 0.85          |
| (2,3)    | 2:205:B:TRP:HE3  | 2:218:B:LEU:HB3  | 8        | 0.85          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD11 | 8        | 0.84          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD12 | 8        | 0.84          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD13 | 8        | 0.84          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD21 | 8        | 0.84          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD22 | 8        | 0.84          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD23 | 8        | 0.84          |
| (2,1231) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HA   | 2        | 0.84          |
| (2,965)  | 1:74:A:PHE:H     | 2:214:B:LEU:HA   | 13       | 0.84          |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3  | 6        | 0.84          |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3  | 6        | 0.84          |
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3  | 6        | 0.84          |
| (1,18)   | 1:53:A:HIS:O     | 1:57:A:SER:H     | 6        | 0.84          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H    | 1        | 0.83          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD11 | 1        | 0.83          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD12 | 1        | 0.83          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD13 | 1        | 0.83          |
| (2,1294) | 2:204:B:THR:HG21 | 2:205:B:TRP:HD1  | 12       | 0.83          |
| (2,1294) | 2:204:B:THR:HG22 | 2:205:B:TRP:HD1  | 12       | 0.83          |
| (2,1294) | 2:204:B:THR:HG23 | 2:205:B:TRP:HD1  | 12       | 0.83          |
| (2,1250) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HG   | 16       | 0.83          |
| (2,1250) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HG   | 16       | 0.83          |
| (2,1231) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HA   | 12       | 0.83          |
| (2,1175) | 2:210:B:SER:HB3  | 2:215:B:LYS:HB3  | 4        | 0.83          |
| (2,752)  | 1:75:A:GLU:H     | 2:214:B:LEU:HG   | 15       | 0.83          |
| (2,632)  | 1:71:A:GLU:HG2   | 2:217:B:ARG:HG2  | 8        | 0.83          |
| (2,3)    | 2:205:B:TRP:HE3  | 2:218:B:LEU:HB3  | 15       | 0.83          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD11 | 4        | 0.82          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD12 | 4        | 0.82          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD13 | 4        | 0.82          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD21 | 4        | 0.82          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD22 | 4        | 0.82          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD23 | 4        | 0.82          |
| (2,1358) | 2:205:B:TRP:HD1  | 2:206:B:ARG:H    | 6        | 0.82          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1126) | 1:70:A:ILE:H     | 2:205:B:TRP:HE3  | 15       | 0.82          |
| (2,11)   | 2:204:B:THR:HA   | 2:205:B:TRP:HD1  | 11       | 0.82          |
| (2,3)    | 2:205:B:TRP:HE3  | 2:218:B:LEU:HB3  | 20       | 0.82          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 4        | 0.82          |
| (1,13)   | 1:51:A:VAL:O     | 1:55:A:ILE:N     | 4        | 0.82          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD11 | 20       | 0.81          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD12 | 20       | 0.81          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD13 | 20       | 0.81          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD21 | 20       | 0.81          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD22 | 20       | 0.81          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD23 | 20       | 0.81          |
| (2,1233) | 2:204:B:THR:HG21 | 2:205:B:TRP:HB3  | 12       | 0.81          |
| (2,1233) | 2:204:B:THR:HG22 | 2:205:B:TRP:HB3  | 12       | 0.81          |
| (2,1233) | 2:204:B:THR:HG23 | 2:205:B:TRP:HB3  | 12       | 0.81          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 2        | 0.81          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 2        | 0.81          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 2        | 0.81          |
| (2,11)   | 2:204:B:THR:HA   | 2:205:B:TRP:HD1  | 12       | 0.81          |
| (1,13)   | 1:51:A:VAL:O     | 1:55:A:ILE:N     | 20       | 0.81          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 1        | 0.8           |
| (2,1144) | 2:205:B:TRP:HZ3  | 2:219:B:THR:HA   | 14       | 0.8           |
| (2,177)  | 1:73:A:ASP:HA    | 2:216:B:ILE:HG21 | 13       | 0.8           |
| (2,177)  | 1:73:A:ASP:HA    | 2:216:B:ILE:HG22 | 13       | 0.8           |
| (2,177)  | 1:73:A:ASP:HA    | 2:216:B:ILE:HG23 | 13       | 0.8           |
| (2,23)   | 1:70:A:ILE:HD11  | 2:205:B:TRP:HH2  | 18       | 0.8           |
| (2,23)   | 1:70:A:ILE:HD12  | 2:205:B:TRP:HH2  | 18       | 0.8           |
| (2,23)   | 1:70:A:ILE:HD13  | 2:205:B:TRP:HH2  | 18       | 0.8           |
| (1,17)   | 1:53:A:HIS:O     | 1:57:A:SER:N     | 6        | 0.8           |
| (2,2150) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG3  | 18       | 0.79          |
| (2,2150) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG3  | 18       | 0.79          |
| (2,1910) | 1:69:A:GLU:HG2   | 2:219:B:THR:HG21 | 14       | 0.79          |
| (2,1910) | 1:69:A:GLU:HG2   | 2:219:B:THR:HG22 | 14       | 0.79          |
| (2,1910) | 1:69:A:GLU:HG2   | 2:219:B:THR:HG23 | 14       | 0.79          |
| (2,1910) | 1:69:A:GLU:HG3   | 2:219:B:THR:HG21 | 14       | 0.79          |
| (2,1910) | 1:69:A:GLU:HG3   | 2:219:B:THR:HG22 | 14       | 0.79          |
| (2,1910) | 1:69:A:GLU:HG3   | 2:219:B:THR:HG23 | 14       | 0.79          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H    | 4        | 0.79          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H    | 10       | 0.79          |
| (2,1455) | 1:74:A:PHE:H     | 2:214:B:LEU:H    | 9        | 0.79          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 14       | 0.79          |
| (2,3)    | 2:205:B:TRP:HE3  | 2:218:B:LEU:HB3  | 13       | 0.79          |
| (1,13)   | 1:51:A:VAL:O     | 1:55:A:ILE:N     | 18       | 0.79          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2230) | 2:220:B:ARG:HD2  | 2:221:B:GLU:H    | 20       | 0.78          |
| (2,2230) | 2:220:B:ARG:HD3  | 2:221:B:GLU:H    | 20       | 0.78          |
| (2,2148) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HB3  | 14       | 0.78          |
| (2,2148) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HB3  | 14       | 0.78          |
| (2,2084) | 2:205:B:TRP:H    | 2:220:B:ARG:HG2  | 1        | 0.78          |
| (2,2084) | 2:205:B:TRP:H    | 2:220:B:ARG:HG3  | 1        | 0.78          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD11 | 14       | 0.78          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD12 | 14       | 0.78          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD13 | 14       | 0.78          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD21 | 14       | 0.78          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD22 | 14       | 0.78          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD23 | 14       | 0.78          |
| (2,616)  | 1:75:A:GLU:HA    | 2:214:B:LEU:HG   | 13       | 0.78          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 20       | 0.78          |
| (2,2172) | 2:210:B:SER:HB2  | 2:215:B:LYS:HD2  | 6        | 0.77          |
| (2,2172) | 2:210:B:SER:HB3  | 2:215:B:LYS:HD2  | 6        | 0.77          |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 6        | 0.77          |
| (2,1475) | 1:73:A:ASP:HA    | 2:216:B:ILE:H    | 19       | 0.77          |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG   | 11       | 0.77          |
| (2,1380) | 2:221:B:GLU:HA   | 2:222:B:ALA:H    | 20       | 0.77          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 9        | 0.77          |
| (2,991)  | 1:70:A:ILE:H     | 2:205:B:TRP:HZ3  | 5        | 0.77          |
| (2,101)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HH2  | 18       | 0.77          |
| (2,101)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HH2  | 18       | 0.77          |
| (2,101)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HH2  | 18       | 0.77          |
| (2,16)   | 2:205:B:TRP:HZ3  | 2:218:B:LEU:HB3  | 12       | 0.77          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD11 | 19       | 0.76          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD12 | 19       | 0.76          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD13 | 19       | 0.76          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD21 | 19       | 0.76          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD22 | 19       | 0.76          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD23 | 19       | 0.76          |
| (2,1242) | 1:70:A:ILE:H     | 2:219:B:THR:HA   | 14       | 0.76          |
| (2,1104) | 1:73:A:ASP:H     | 2:215:B:LYS:HA   | 13       | 0.76          |
| (2,176)  | 1:73:A:ASP:HA    | 2:215:B:LYS:HD3  | 2        | 0.76          |
| (2,14)   | 1:70:A:ILE:HD11  | 2:205:B:TRP:HZ3  | 8        | 0.76          |
| (2,14)   | 1:70:A:ILE:HD12  | 2:205:B:TRP:HZ3  | 8        | 0.76          |
| (2,14)   | 1:70:A:ILE:HD13  | 2:205:B:TRP:HZ3  | 8        | 0.76          |
| (1,17)   | 1:53:A:HIS:O     | 1:57:A:SER:N     | 3        | 0.76          |
| (2,1455) | 1:74:A:PHE:H     | 2:214:B:LEU:H    | 13       | 0.75          |
| (2,1426) | 2:214:B:LEU:H    | 2:215:B:LYS:HG3  | 10       | 0.75          |
| (2,1383) | 2:206:B:ARG:H    | 2:220:B:ARG:HA   | 1        | 0.75          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 8        | 0.75          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 11       | 0.75          |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3  | 16       | 0.75          |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3  | 16       | 0.75          |
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3  | 16       | 0.75          |
| (2,1908) | 1:69:A:GLU:HG2   | 2:217:B:ARG:HD2  | 10       | 0.74          |
| (2,1908) | 1:69:A:GLU:HG2   | 2:217:B:ARG:HD3  | 10       | 0.74          |
| (2,1908) | 1:69:A:GLU:HG3   | 2:217:B:ARG:HD2  | 10       | 0.74          |
| (2,1908) | 1:69:A:GLU:HG3   | 2:217:B:ARG:HD3  | 10       | 0.74          |
| (2,1477) | 2:208:B:GLN:HE22 | 2:219:B:THR:HG21 | 20       | 0.74          |
| (2,1477) | 2:208:B:GLN:HE22 | 2:219:B:THR:HG22 | 20       | 0.74          |
| (2,1477) | 2:208:B:GLN:HE22 | 2:219:B:THR:HG23 | 20       | 0.74          |
| (2,1367) | 1:73:A:ASP:HA    | 2:215:B:LYS:H    | 9        | 0.74          |
| (2,1243) | 2:205:B:TRP:HA   | 2:220:B:ARG:HG2  | 1        | 0.74          |
| (2,615)  | 1:75:A:GLU:HG2   | 2:214:B:LEU:HB2  | 14       | 0.74          |
| (2,1484) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HG3  | 2        | 0.73          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 19       | 0.73          |
| (2,1242) | 1:70:A:ILE:H     | 2:219:B:THR:HA   | 9        | 0.73          |
| (2,615)  | 1:75:A:GLU:HG2   | 2:214:B:LEU:HB2  | 13       | 0.73          |
| (2,531)  | 1:76:A:THR:HG21  | 2:215:B:LYS:HD3  | 11       | 0.73          |
| (2,531)  | 1:76:A:THR:HG22  | 2:215:B:LYS:HD3  | 11       | 0.73          |
| (2,531)  | 1:76:A:THR:HG23  | 2:215:B:LYS:HD3  | 11       | 0.73          |
| (2,176)  | 1:73:A:ASP:HA    | 2:215:B:LYS:HD3  | 10       | 0.73          |
| (2,11)   | 2:204:B:THR:HA   | 2:205:B:TRP:HD1  | 8        | 0.73          |
| (1,18)   | 1:53:A:HIS:O     | 1:57:A:SER:H     | 3        | 0.73          |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H    | 15       | 0.72          |
| (2,1145) | 2:205:B:TRP:HE3  | 2:219:B:THR:HA   | 1        | 0.72          |
| (2,1145) | 2:205:B:TRP:HE3  | 2:219:B:THR:HA   | 5        | 0.72          |
| (2,28)   | 1:69:A:GLU:HA    | 2:205:B:TRP:HZ3  | 16       | 0.72          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 18       | 0.72          |
| (1,13)   | 1:51:A:VAL:O     | 1:55:A:ILE:N     | 8        | 0.72          |
| (2,2163) | 2:209:B:ARG:HG2  | 2:210:B:SER:HA   | 9        | 0.71          |
| (2,2163) | 2:209:B:ARG:HG3  | 2:210:B:SER:HA   | 9        | 0.71          |
| (2,2111) | 2:206:B:ARG:HG2  | 2:221:B:GLU:HG2  | 11       | 0.71          |
| (2,2111) | 2:206:B:ARG:HG2  | 2:221:B:GLU:HG3  | 11       | 0.71          |
| (2,2111) | 2:206:B:ARG:HG3  | 2:221:B:GLU:HG2  | 11       | 0.71          |
| (2,2111) | 2:206:B:ARG:HG3  | 2:221:B:GLU:HG3  | 11       | 0.71          |
| (2,2110) | 2:206:B:ARG:HG2  | 2:221:B:GLU:H    | 11       | 0.71          |
| (2,2110) | 2:206:B:ARG:HG3  | 2:221:B:GLU:H    | 11       | 0.71          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD11 | 16       | 0.71          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD12 | 16       | 0.71          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD13 | 16       | 0.71          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD21 | 16       | 0.71          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD22 | 16       | 0.71          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD23 | 16       | 0.71          |
| (2,1955) | 1:75:A:GLU:HG3  | 2:214:B:LEU:HD11 | 12       | 0.71          |
| (2,1955) | 1:75:A:GLU:HG3  | 2:214:B:LEU:HD12 | 12       | 0.71          |
| (2,1955) | 1:75:A:GLU:HG3  | 2:214:B:LEU:HD13 | 12       | 0.71          |
| (2,1955) | 1:75:A:GLU:HG3  | 2:214:B:LEU:HD21 | 12       | 0.71          |
| (2,1955) | 1:75:A:GLU:HG3  | 2:214:B:LEU:HD22 | 12       | 0.71          |
| (2,1955) | 1:75:A:GLU:HG3  | 2:214:B:LEU:HD23 | 12       | 0.71          |
| (2,1929) | 1:73:A:ASP:HB2  | 2:215:B:LYS:HA   | 14       | 0.71          |
| (2,1929) | 1:73:A:ASP:HB3  | 2:215:B:LYS:HA   | 14       | 0.71          |
| (2,1251) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HG   | 6        | 0.71          |
| (2,1243) | 2:205:B:TRP:HA  | 2:220:B:ARG:HG2  | 8        | 0.71          |
| (2,1218) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD21 | 15       | 0.71          |
| (2,1218) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD22 | 15       | 0.71          |
| (2,1218) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD23 | 15       | 0.71          |
| (2,1150) | 2:217:B:ARG:HG2 | 2:219:B:THR:HG21 | 7        | 0.71          |
| (2,1150) | 2:217:B:ARG:HG2 | 2:219:B:THR:HG22 | 7        | 0.71          |
| (2,1150) | 2:217:B:ARG:HG2 | 2:219:B:THR:HG23 | 7        | 0.71          |
| (2,801)  | 1:74:A:PHE:H    | 2:214:B:LEU:HB2  | 13       | 0.71          |
| (2,536)  | 1:74:A:PHE:HB2  | 2:214:B:LEU:HD11 | 13       | 0.71          |
| (2,536)  | 1:74:A:PHE:HB2  | 2:214:B:LEU:HD12 | 13       | 0.71          |
| (2,536)  | 1:74:A:PHE:HB2  | 2:214:B:LEU:HD13 | 13       | 0.71          |
| (2,208)  | 1:69:A:GLU:HA   | 2:205:B:TRP:HE3  | 2        | 0.71          |
| (2,162)  | 1:52:A:VAL:HG11 | 2:205:B:TRP:HZ3  | 20       | 0.71          |
| (2,162)  | 1:52:A:VAL:HG12 | 2:205:B:TRP:HZ3  | 20       | 0.71          |
| (2,162)  | 1:52:A:VAL:HG13 | 2:205:B:TRP:HZ3  | 20       | 0.71          |
| (2,11)   | 2:204:B:THR:HA  | 2:205:B:TRP:HD1  | 5        | 0.71          |
| (1,13)   | 1:51:A:VAL:O    | 1:55:A:ILE:N     | 13       | 0.71          |
| (1,13)   | 1:51:A:VAL:O    | 1:55:A:ILE:N     | 17       | 0.71          |
| (2,2118) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD11 | 12       | 0.7           |
| (2,2118) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD12 | 12       | 0.7           |
| (2,2118) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD13 | 12       | 0.7           |
| (2,2118) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD21 | 12       | 0.7           |
| (2,2118) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD22 | 12       | 0.7           |
| (2,2118) | 2:207:B:VAL:HB  | 2:218:B:LEU:HD23 | 12       | 0.7           |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD11 | 8        | 0.7           |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD12 | 8        | 0.7           |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD13 | 8        | 0.7           |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD21 | 8        | 0.7           |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD22 | 8        | 0.7           |
| (2,2097) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HD23 | 8        | 0.7           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1331) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD21 | 12       | 0.7           |
| (2,1331) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD22 | 12       | 0.7           |
| (2,1331) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD23 | 12       | 0.7           |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 6        | 0.7           |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 6        | 0.7           |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 6        | 0.7           |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD11 | 5        | 0.7           |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD12 | 5        | 0.7           |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD13 | 5        | 0.7           |
| (2,1169) | 1:74:A:PHE:HB2   | 2:214:B:LEU:HB2  | 9        | 0.7           |
| (2,160)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ3  | 17       | 0.7           |
| (2,160)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ3  | 17       | 0.7           |
| (2,160)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ3  | 17       | 0.7           |
| (1,13)   | 1:51:A:VAL:O     | 1:55:A:ILE:N     | 1        | 0.7           |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD11 | 8        | 0.69          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD12 | 8        | 0.69          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD13 | 8        | 0.69          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD21 | 8        | 0.69          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD22 | 8        | 0.69          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD23 | 8        | 0.69          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD11 | 14       | 0.69          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD12 | 14       | 0.69          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD13 | 14       | 0.69          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD21 | 14       | 0.69          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD22 | 14       | 0.69          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD23 | 14       | 0.69          |
| (2,1908) | 1:69:A:GLU:HG2   | 2:217:B:ARG:HD2  | 16       | 0.69          |
| (2,1908) | 1:69:A:GLU:HG2   | 2:217:B:ARG:HD3  | 16       | 0.69          |
| (2,1908) | 1:69:A:GLU:HG3   | 2:217:B:ARG:HD2  | 16       | 0.69          |
| (2,1908) | 1:69:A:GLU:HG3   | 2:217:B:ARG:HD3  | 16       | 0.69          |
| (2,1736) | 1:48:A:LEU:HD11  | 2:205:B:TRP:H    | 16       | 0.69          |
| (2,1736) | 1:48:A:LEU:HD12  | 2:205:B:TRP:H    | 16       | 0.69          |
| (2,1736) | 1:48:A:LEU:HD13  | 2:205:B:TRP:H    | 16       | 0.69          |
| (2,1736) | 1:48:A:LEU:HD21  | 2:205:B:TRP:H    | 16       | 0.69          |
| (2,1736) | 1:48:A:LEU:HD22  | 2:205:B:TRP:H    | 16       | 0.69          |
| (2,1736) | 1:48:A:LEU:HD23  | 2:205:B:TRP:H    | 16       | 0.69          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 17       | 0.69          |
| (2,1257) | 1:73:A:ASP:HA    | 2:215:B:LYS:HB2  | 11       | 0.69          |
| (2,1250) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HG   | 6        | 0.69          |
| (2,1250) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HG   | 6        | 0.69          |
| (2,2127) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HG   | 3        | 0.68          |
| (2,2127) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HG   | 3        | 0.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2127) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HG   | 3        | 0.68          |
| (2,2127) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HG   | 3        | 0.68          |
| (2,2127) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HG   | 3        | 0.68          |
| (2,2127) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HG   | 3        | 0.68          |
| (2,1932) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HD3  | 12       | 0.68          |
| (2,1932) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HD3  | 12       | 0.68          |
| (2,1367) | 1:73:A:ASP:HA    | 2:215:B:LYS:H    | 14       | 0.68          |
| (2,1257) | 1:73:A:ASP:HA    | 2:215:B:LYS:HB2  | 20       | 0.68          |
| (2,1253) | 2:214:B:LEU:HG   | 2:215:B:LYS:H    | 12       | 0.68          |
| (2,1224) | 1:70:A:ILE:HD11  | 2:219:B:THR:HA   | 15       | 0.68          |
| (2,1224) | 1:70:A:ILE:HD12  | 2:219:B:THR:HA   | 15       | 0.68          |
| (2,1224) | 1:70:A:ILE:HD13  | 2:219:B:THR:HA   | 15       | 0.68          |
| (2,1171) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HB2  | 9        | 0.68          |
| (1,1)    | 1:33:A:LYS:O     | 1:37:A:SER:N     | 7        | 0.68          |
| (2,2150) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG3  | 3        | 0.67          |
| (2,2150) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG3  | 3        | 0.67          |
| (2,1486) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB3  | 6        | 0.67          |
| (2,1418) | 2:214:B:LEU:H    | 2:215:B:LYS:HB2  | 2        | 0.67          |
| (2,1174) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HB2  | 14       | 0.67          |
| (2,636)  | 1:69:A:GLU:HA    | 2:219:B:THR:HG21 | 1        | 0.67          |
| (2,636)  | 1:69:A:GLU:HA    | 2:219:B:THR:HG22 | 1        | 0.67          |
| (2,636)  | 1:69:A:GLU:HA    | 2:219:B:THR:HG23 | 1        | 0.67          |
| (2,177)  | 1:73:A:ASP:HA    | 2:216:B:ILE:HG21 | 15       | 0.67          |
| (2,177)  | 1:73:A:ASP:HA    | 2:216:B:ILE:HG22 | 15       | 0.67          |
| (2,177)  | 1:73:A:ASP:HA    | 2:216:B:ILE:HG23 | 15       | 0.67          |
| (2,11)   | 2:204:B:THR:HA   | 2:205:B:TRP:HD1  | 18       | 0.67          |
| (1,22)   | 1:87:A:ARG:O     | 1:91:A:SER:H     | 5        | 0.67          |
| (1,2)    | 1:33:A:LYS:O     | 1:37:A:SER:H     | 6        | 0.67          |
| (2,1459) | 2:220:B:ARG:HD2  | 2:221:B:GLU:H    | 20       | 0.66          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 7        | 0.66          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 7        | 0.66          |
| (2,1218) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 7        | 0.66          |
| (2,720)  | 1:74:A:PHE:H     | 2:215:B:LYS:HG2  | 11       | 0.66          |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3  | 1        | 0.66          |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3  | 1        | 0.66          |
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3  | 1        | 0.66          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 16       | 0.66          |
| (2,11)   | 2:204:B:THR:HA   | 2:205:B:TRP:HD1  | 2        | 0.66          |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 3        | 0.66          |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 6        | 0.66          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD11 | 4        | 0.65          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD12 | 4        | 0.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD13 | 4        | 0.65          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD21 | 4        | 0.65          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD22 | 4        | 0.65          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD23 | 4        | 0.65          |
| (2,1397) | 2:205:B:TRP:HB2  | 2:220:B:ARG:H    | 1        | 0.65          |
| (2,1294) | 2:204:B:THR:HG21 | 2:205:B:TRP:HD1  | 3        | 0.65          |
| (2,1294) | 2:204:B:THR:HG22 | 2:205:B:TRP:HD1  | 3        | 0.65          |
| (2,1294) | 2:204:B:THR:HG23 | 2:205:B:TRP:HD1  | 3        | 0.65          |
| (2,1243) | 2:205:B:TRP:HA   | 2:220:B:ARG:HG2  | 10       | 0.65          |
| (2,1175) | 2:210:B:SER:HB3  | 2:215:B:LYS:HB3  | 9        | 0.65          |
| (2,1164) | 1:71:A:GLU:HG3   | 2:217:B:ARG:HB2  | 10       | 0.65          |
| (2,1152) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HA   | 14       | 0.65          |
| (2,1152) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HA   | 14       | 0.65          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 1        | 0.65          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 8        | 0.65          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD11 | 20       | 0.64          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD12 | 20       | 0.64          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD13 | 20       | 0.64          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD21 | 20       | 0.64          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD22 | 20       | 0.64          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD23 | 20       | 0.64          |
| (2,1407) | 2:213:B:PRO:HG2  | 2:214:B:LEU:H    | 1        | 0.64          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 13       | 0.64          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 20       | 0.64          |
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 5        | 0.64          |
| (2,1242) | 1:70:A:ILE:H     | 2:219:B:THR:HA   | 1        | 0.64          |
| (2,1225) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HA   | 9        | 0.64          |
| (1,21)   | 1:87:A:ARG:O     | 1:91:A:SER:N     | 5        | 0.64          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 13       | 0.64          |
| (1,1)    | 1:33:A:LYS:O     | 1:37:A:SER:N     | 6        | 0.64          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD11 | 1        | 0.63          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD12 | 1        | 0.63          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD13 | 1        | 0.63          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD21 | 1        | 0.63          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD22 | 1        | 0.63          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD23 | 1        | 0.63          |
| (2,2094) | 2:205:B:TRP:HE3  | 2:220:B:ARG:HB2  | 6        | 0.63          |
| (2,2094) | 2:205:B:TRP:HE3  | 2:220:B:ARG:HB3  | 6        | 0.63          |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 11       | 0.63          |
| (2,1227) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HA   | 13       | 0.63          |
| (2,636)  | 1:69:A:GLU:HA    | 2:219:B:THR:HG21 | 14       | 0.63          |
| (2,636)  | 1:69:A:GLU:HA    | 2:219:B:THR:HG22 | 14       | 0.63          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,636)  | 1:69:A:GLU:HA   | 2:219:B:THR:HG23 | 14       | 0.63          |
| (2,615)  | 1:75:A:GLU:HG2  | 2:214:B:LEU:HB2  | 15       | 0.63          |
| (1,14)   | 1:51:A:VAL:O    | 1:55:A:ILE:H     | 17       | 0.63          |
| (1,2)    | 1:33:A:LYS:O    | 1:37:A:SER:H     | 7        | 0.63          |
| (2,1602) | 1:34:A:ARG:HG3  | 2:213:B:PRO:HB2  | 18       | 0.62          |
| (2,1602) | 1:34:A:ARG:HG3  | 2:213:B:PRO:HB3  | 18       | 0.62          |
| (2,1270) | 2:203:B:LEU:HB3 | 2:204:B:THR:HB   | 12       | 0.62          |
| (2,1248) | 1:74:A:PHE:H    | 2:214:B:LEU:HD11 | 13       | 0.62          |
| (2,1248) | 1:74:A:PHE:H    | 2:214:B:LEU:HD12 | 13       | 0.62          |
| (2,1248) | 1:74:A:PHE:H    | 2:214:B:LEU:HD13 | 13       | 0.62          |
| (1,22)   | 1:87:A:ARG:O    | 1:91:A:SER:H     | 4        | 0.62          |
| (2,2189) | 2:213:B:PRO:HA  | 2:214:B:LEU:HD11 | 9        | 0.61          |
| (2,2189) | 2:213:B:PRO:HA  | 2:214:B:LEU:HD12 | 9        | 0.61          |
| (2,2189) | 2:213:B:PRO:HA  | 2:214:B:LEU:HD13 | 9        | 0.61          |
| (2,2189) | 2:213:B:PRO:HA  | 2:214:B:LEU:HD21 | 9        | 0.61          |
| (2,2189) | 2:213:B:PRO:HA  | 2:214:B:LEU:HD22 | 9        | 0.61          |
| (2,2189) | 2:213:B:PRO:HA  | 2:214:B:LEU:HD23 | 9        | 0.61          |
| (2,2094) | 2:205:B:TRP:HE3 | 2:220:B:ARG:HB2  | 5        | 0.61          |
| (2,2094) | 2:205:B:TRP:HE3 | 2:220:B:ARG:HB3  | 5        | 0.61          |
| (2,1954) | 1:75:A:GLU:HG2  | 2:214:B:LEU:HD11 | 12       | 0.61          |
| (2,1954) | 1:75:A:GLU:HG2  | 2:214:B:LEU:HD12 | 12       | 0.61          |
| (2,1954) | 1:75:A:GLU:HG2  | 2:214:B:LEU:HD13 | 12       | 0.61          |
| (2,1954) | 1:75:A:GLU:HG2  | 2:214:B:LEU:HD21 | 12       | 0.61          |
| (2,1954) | 1:75:A:GLU:HG2  | 2:214:B:LEU:HD22 | 12       | 0.61          |
| (2,1954) | 1:75:A:GLU:HG2  | 2:214:B:LEU:HD23 | 12       | 0.61          |
| (2,1355) | 1:74:A:PHE:HD1  | 2:214:B:LEU:H    | 3        | 0.61          |
| (2,1355) | 1:74:A:PHE:HD2  | 2:214:B:LEU:H    | 3        | 0.61          |
| (2,1137) | 1:70:A:ILE:H    | 2:219:B:THR:HG21 | 7        | 0.61          |
| (2,1137) | 1:70:A:ILE:H    | 2:219:B:THR:HG22 | 7        | 0.61          |
| (2,1137) | 1:70:A:ILE:H    | 2:219:B:THR:HG23 | 7        | 0.61          |
| (2,616)  | 1:75:A:GLU:HA   | 2:214:B:LEU:HG   | 15       | 0.61          |
| (2,531)  | 1:76:A:THR:HG21 | 2:215:B:LYS:HD3  | 8        | 0.61          |
| (2,531)  | 1:76:A:THR:HG22 | 2:215:B:LYS:HD3  | 8        | 0.61          |
| (2,531)  | 1:76:A:THR:HG23 | 2:215:B:LYS:HD3  | 8        | 0.61          |
| (2,2230) | 2:220:B:ARG:HD2 | 2:221:B:GLU:H    | 18       | 0.6           |
| (2,2230) | 2:220:B:ARG:HD3 | 2:221:B:GLU:H    | 18       | 0.6           |
| (2,1605) | 1:34:A:ARG:HD2  | 2:213:B:PRO:HB2  | 15       | 0.6           |
| (2,1605) | 1:34:A:ARG:HD2  | 2:213:B:PRO:HB3  | 15       | 0.6           |
| (2,1605) | 1:34:A:ARG:HD3  | 2:213:B:PRO:HB2  | 15       | 0.6           |
| (2,1605) | 1:34:A:ARG:HD3  | 2:213:B:PRO:HB3  | 15       | 0.6           |
| (2,1333) | 1:34:A:ARG:HG2  | 2:213:B:PRO:HG3  | 3        | 0.6           |
| (2,143)  | 1:70:A:ILE:HG13 | 2:205:B:TRP:HH2  | 6        | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,95)   | 1:74:A:PHE:HB2   | 2:214:B:LEU:HA   | 13       | 0.6           |
| (1,13)   | 1:51:A:VAL:O     | 1:55:A:ILE:N     | 6        | 0.6           |
| (1,12)   | 1:50:A:ARG:O     | 1:54:A:ILE:H     | 3        | 0.6           |
| (1,5)    | 1:35:A:GLN:O     | 1:39:A:ASP:N     | 1        | 0.6           |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 3        | 0.59          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H    | 11       | 0.59          |
| (2,1407) | 2:213:B:PRO:HG2  | 2:214:B:LEU:H    | 5        | 0.59          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 4        | 0.59          |
| (2,1273) | 2:220:B:ARG:HD3  | 2:221:B:GLU:H    | 20       | 0.59          |
| (2,1267) | 2:205:B:TRP:HE3  | 2:220:B:ARG:HB3  | 8        | 0.59          |
| (2,1251) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HG   | 5        | 0.59          |
| (2,1250) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HG   | 3        | 0.59          |
| (2,1250) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HG   | 3        | 0.59          |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG21 | 11       | 0.59          |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG22 | 11       | 0.59          |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG23 | 11       | 0.59          |
| (2,160)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ3  | 18       | 0.59          |
| (2,160)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ3  | 18       | 0.59          |
| (2,160)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ3  | 18       | 0.59          |
| (1,21)   | 1:87:A:ARG:O     | 1:91:A:SER:N     | 4        | 0.59          |
| (2,2149) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG2  | 7        | 0.58          |
| (2,2149) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG2  | 7        | 0.58          |
| (2,2083) | 2:204:B:THR:H    | 2:220:B:ARG:HD2  | 1        | 0.58          |
| (2,2083) | 2:204:B:THR:H    | 2:220:B:ARG:HD3  | 1        | 0.58          |
| (2,2076) | 2:203:B:LEU:HA   | 2:220:B:ARG:HD2  | 1        | 0.58          |
| (2,2076) | 2:203:B:LEU:HA   | 2:220:B:ARG:HD3  | 1        | 0.58          |
| (2,1932) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HD3  | 10       | 0.58          |
| (2,1932) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HD3  | 10       | 0.58          |
| (2,1319) | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD21 | 8        | 0.58          |
| (2,1319) | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD22 | 8        | 0.58          |
| (2,1319) | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD23 | 8        | 0.58          |
| (2,1267) | 2:205:B:TRP:HE3  | 2:220:B:ARG:HB3  | 13       | 0.58          |
| (2,1202) | 2:215:B:LYS:HG2  | 2:216:B:ILE:H    | 2        | 0.58          |
| (2,1178) | 2:210:B:SER:HB3  | 2:215:B:LYS:HB2  | 12       | 0.58          |
| (2,13)   | 1:70:A:ILE:HG12  | 2:205:B:TRP:HZ3  | 2        | 0.58          |
| (2,3)    | 2:205:B:TRP:HE3  | 2:218:B:LEU:HB3  | 11       | 0.58          |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 9        | 0.58          |
| (2,2199) | 2:214:B:LEU:HD11 | 2:215:B:LYS:H    | 16       | 0.57          |
| (2,2199) | 2:214:B:LEU:HD12 | 2:215:B:LYS:H    | 16       | 0.57          |
| (2,2199) | 2:214:B:LEU:HD13 | 2:215:B:LYS:H    | 16       | 0.57          |
| (2,2199) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H    | 16       | 0.57          |
| (2,2199) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H    | 16       | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2199) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H    | 16       | 0.57          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD11 | 14       | 0.57          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD12 | 14       | 0.57          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD13 | 14       | 0.57          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 14       | 0.57          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 14       | 0.57          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 14       | 0.57          |
| (2,2113) | 2:206:B:ARG:HD2  | 2:221:B:GLU:HG2  | 2        | 0.57          |
| (2,2113) | 2:206:B:ARG:HD2  | 2:221:B:GLU:HG3  | 2        | 0.57          |
| (2,2113) | 2:206:B:ARG:HD3  | 2:221:B:GLU:HG2  | 2        | 0.57          |
| (2,2113) | 2:206:B:ARG:HD3  | 2:221:B:GLU:HG3  | 2        | 0.57          |
| (2,1795) | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ2  | 4        | 0.57          |
| (2,1795) | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ2  | 4        | 0.57          |
| (2,1795) | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ2  | 4        | 0.57          |
| (2,1795) | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ2  | 4        | 0.57          |
| (2,1795) | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ2  | 4        | 0.57          |
| (2,1795) | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ2  | 4        | 0.57          |
| (2,1479) | 2:208:B:GLN:HE21 | 2:219:B:THR:HB   | 19       | 0.57          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H    | 16       | 0.57          |
| (2,1340) | 2:205:B:TRP:HE3  | 2:219:B:THR:H    | 1        | 0.57          |
| (2,531)  | 1:76:A:THR:HG21  | 2:215:B:LYS:HD3  | 7        | 0.57          |
| (2,531)  | 1:76:A:THR:HG22  | 2:215:B:LYS:HD3  | 7        | 0.57          |
| (2,531)  | 1:76:A:THR:HG23  | 2:215:B:LYS:HD3  | 7        | 0.57          |
| (2,95)   | 1:74:A:PHE:HB2   | 2:214:B:LEU:HA   | 15       | 0.57          |
| (2,14)   | 1:70:A:ILE:HD11  | 2:205:B:TRP:HZ3  | 18       | 0.57          |
| (2,14)   | 1:70:A:ILE:HD12  | 2:205:B:TRP:HZ3  | 18       | 0.57          |
| (2,14)   | 1:70:A:ILE:HD13  | 2:205:B:TRP:HZ3  | 18       | 0.57          |
| (2,2110) | 2:206:B:ARG:HG2  | 2:221:B:GLU:H    | 14       | 0.56          |
| (2,2110) | 2:206:B:ARG:HG3  | 2:221:B:GLU:H    | 14       | 0.56          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD11 | 6        | 0.56          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD12 | 6        | 0.56          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD13 | 6        | 0.56          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD21 | 6        | 0.56          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD22 | 6        | 0.56          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD23 | 6        | 0.56          |
| (2,1929) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HA   | 15       | 0.56          |
| (2,1929) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HA   | 15       | 0.56          |
| (2,1486) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB3  | 13       | 0.56          |
| (2,1406) | 2:214:B:LEU:HB2  | 2:215:B:LYS:H    | 3        | 0.56          |
| (2,1383) | 2:206:B:ARG:H    | 2:220:B:ARG:HA   | 10       | 0.56          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 3        | 0.56          |
| (2,1163) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HB3  | 2        | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,30)   | 1:30:A:TYR:HE1   | 2:214:B:LEU:HG   | 9        | 0.56          |
| (2,30)   | 1:30:A:TYR:HE2   | 2:214:B:LEU:HG   | 9        | 0.56          |
| (2,15)   | 1:70:A:ILE:HG13  | 2:205:B:TRP:HZ3  | 20       | 0.56          |
| (1,12)   | 1:50:A:ARG:O     | 1:54:A:ILE:H     | 6        | 0.56          |
| (2,2199) | 2:214:B:LEU:HD11 | 2:215:B:LYS:H    | 6        | 0.55          |
| (2,2199) | 2:214:B:LEU:HD12 | 2:215:B:LYS:H    | 6        | 0.55          |
| (2,2199) | 2:214:B:LEU:HD13 | 2:215:B:LYS:H    | 6        | 0.55          |
| (2,2199) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H    | 6        | 0.55          |
| (2,2199) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H    | 6        | 0.55          |
| (2,2199) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H    | 6        | 0.55          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE2  | 6        | 0.55          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE3  | 6        | 0.55          |
| (2,2184) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HB3  | 10       | 0.55          |
| (2,2184) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB3  | 10       | 0.55          |
| (2,2140) | 2:208:B:GLN:HB2  | 2:217:B:ARG:HD2  | 20       | 0.55          |
| (2,2140) | 2:208:B:GLN:HB2  | 2:217:B:ARG:HD3  | 20       | 0.55          |
| (2,2140) | 2:208:B:GLN:HB3  | 2:217:B:ARG:HD2  | 20       | 0.55          |
| (2,2140) | 2:208:B:GLN:HB3  | 2:217:B:ARG:HD3  | 20       | 0.55          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD11 | 14       | 0.55          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD12 | 14       | 0.55          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD13 | 14       | 0.55          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD21 | 14       | 0.55          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD22 | 14       | 0.55          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD23 | 14       | 0.55          |
| (2,1744) | 1:48:A:LEU:HD11  | 2:218:B:LEU:HG   | 11       | 0.55          |
| (2,1744) | 1:48:A:LEU:HD12  | 2:218:B:LEU:HG   | 11       | 0.55          |
| (2,1744) | 1:48:A:LEU:HD13  | 2:218:B:LEU:HG   | 11       | 0.55          |
| (2,1744) | 1:48:A:LEU:HD21  | 2:218:B:LEU:HG   | 11       | 0.55          |
| (2,1744) | 1:48:A:LEU:HD22  | 2:218:B:LEU:HG   | 11       | 0.55          |
| (2,1744) | 1:48:A:LEU:HD23  | 2:218:B:LEU:HG   | 11       | 0.55          |
| (2,1488) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HD3  | 1        | 0.55          |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 1        | 0.55          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H    | 8        | 0.55          |
| (2,1386) | 2:204:B:THR:HB   | 2:205:B:TRP:H    | 8        | 0.55          |
| (2,1353) | 1:74:A:PHE:HD1   | 2:215:B:LYS:H    | 10       | 0.55          |
| (2,1353) | 1:74:A:PHE:HD2   | 2:215:B:LYS:H    | 10       | 0.55          |
| (2,1202) | 2:215:B:LYS:HG2  | 2:216:B:ILE:H    | 11       | 0.55          |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 18       | 0.55          |
| (2,2187) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE2  | 20       | 0.54          |
| (2,2187) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE3  | 20       | 0.54          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD11 | 16       | 0.54          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD12 | 16       | 0.54          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1943) | 1:74:A:PHE:HD1  | 2:214:B:LEU:HD13 | 16       | 0.54          |
| (2,1943) | 1:74:A:PHE:HD1  | 2:214:B:LEU:HD21 | 16       | 0.54          |
| (2,1943) | 1:74:A:PHE:HD1  | 2:214:B:LEU:HD22 | 16       | 0.54          |
| (2,1943) | 1:74:A:PHE:HD1  | 2:214:B:LEU:HD23 | 16       | 0.54          |
| (2,1943) | 1:74:A:PHE:HD2  | 2:214:B:LEU:HD11 | 16       | 0.54          |
| (2,1943) | 1:74:A:PHE:HD2  | 2:214:B:LEU:HD12 | 16       | 0.54          |
| (2,1943) | 1:74:A:PHE:HD2  | 2:214:B:LEU:HD13 | 16       | 0.54          |
| (2,1943) | 1:74:A:PHE:HD2  | 2:214:B:LEU:HD21 | 16       | 0.54          |
| (2,1943) | 1:74:A:PHE:HD2  | 2:214:B:LEU:HD22 | 16       | 0.54          |
| (2,1943) | 1:74:A:PHE:HD2  | 2:214:B:LEU:HD23 | 16       | 0.54          |
| (2,1606) | 1:34:A:ARG:HD2  | 2:213:B:PRO:HG3  | 8        | 0.54          |
| (2,1606) | 1:34:A:ARG:HD3  | 2:213:B:PRO:HG3  | 8        | 0.54          |
| (2,1474) | 1:75:A:GLU:HG2  | 2:215:B:LYS:H    | 12       | 0.54          |
| (2,1403) | 2:221:B:GLU:HB3 | 2:222:B:ALA:H    | 8        | 0.54          |
| (2,1397) | 2:205:B:TRP:HB2 | 2:220:B:ARG:H    | 8        | 0.54          |
| (2,1386) | 2:204:B:THR:HB  | 2:205:B:TRP:H    | 16       | 0.54          |
| (2,1164) | 1:71:A:GLU:HG3  | 2:217:B:ARG:HB2  | 16       | 0.54          |
| (2,1163) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HB3  | 15       | 0.54          |
| (2,1144) | 2:205:B:TRP:HZ3 | 2:219:B:THR:HA   | 7        | 0.54          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD11 | 2        | 0.53          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD12 | 2        | 0.53          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD13 | 2        | 0.53          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD21 | 2        | 0.53          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD22 | 2        | 0.53          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD23 | 2        | 0.53          |
| (2,1955) | 1:75:A:GLU:HG3  | 2:214:B:LEU:HD11 | 18       | 0.53          |
| (2,1955) | 1:75:A:GLU:HG3  | 2:214:B:LEU:HD12 | 18       | 0.53          |
| (2,1955) | 1:75:A:GLU:HG3  | 2:214:B:LEU:HD13 | 18       | 0.53          |
| (2,1955) | 1:75:A:GLU:HG3  | 2:214:B:LEU:HD21 | 18       | 0.53          |
| (2,1955) | 1:75:A:GLU:HG3  | 2:214:B:LEU:HD22 | 18       | 0.53          |
| (2,1955) | 1:75:A:GLU:HG3  | 2:214:B:LEU:HD23 | 18       | 0.53          |
| (2,1931) | 1:73:A:ASP:HB2  | 2:215:B:LYS:HG3  | 19       | 0.53          |
| (2,1931) | 1:73:A:ASP:HB3  | 2:215:B:LYS:HG3  | 19       | 0.53          |
| (2,1602) | 1:34:A:ARG:HG3  | 2:213:B:PRO:HB2  | 14       | 0.53          |
| (2,1602) | 1:34:A:ARG:HG3  | 2:213:B:PRO:HB3  | 14       | 0.53          |
| (2,1455) | 1:74:A:PHE:H    | 2:214:B:LEU:H    | 15       | 0.53          |
| (2,1452) | 1:71:A:GLU:HG2  | 2:218:B:LEU:H    | 8        | 0.53          |
| (2,1386) | 2:204:B:THR:HB  | 2:205:B:TRP:H    | 14       | 0.53          |
| (2,1265) | 2:204:B:THR:HB  | 2:205:B:TRP:HB3  | 16       | 0.53          |
| (2,619)  | 1:72:A:ILE:HB   | 2:216:B:ILE:HB   | 13       | 0.53          |
| (2,160)  | 1:52:A:VAL:HG21 | 2:205:B:TRP:HZ3  | 8        | 0.53          |
| (2,160)  | 1:52:A:VAL:HG22 | 2:205:B:TRP:HZ3  | 8        | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,160)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ3  | 8        | 0.53          |
| (2,101)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HH2  | 8        | 0.53          |
| (2,101)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HH2  | 8        | 0.53          |
| (2,101)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HH2  | 8        | 0.53          |
| (2,95)   | 1:74:A:PHE:HB2   | 2:214:B:LEU:HA   | 9        | 0.53          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 6        | 0.53          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 11       | 0.53          |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H     | 11       | 0.53          |
| (2,2124) | 2:207:B:VAL:HG11 | 2:218:B:LEU:H    | 19       | 0.52          |
| (2,2124) | 2:207:B:VAL:HG12 | 2:218:B:LEU:H    | 19       | 0.52          |
| (2,2124) | 2:207:B:VAL:HG13 | 2:218:B:LEU:H    | 19       | 0.52          |
| (2,2124) | 2:207:B:VAL:HG21 | 2:218:B:LEU:H    | 19       | 0.52          |
| (2,2124) | 2:207:B:VAL:HG22 | 2:218:B:LEU:H    | 19       | 0.52          |
| (2,2124) | 2:207:B:VAL:HG23 | 2:218:B:LEU:H    | 19       | 0.52          |
| (2,1465) | 2:205:B:TRP:HE3  | 2:221:B:GLU:H    | 6        | 0.52          |
| (2,1386) | 2:204:B:THR:HB   | 2:205:B:TRP:H    | 3        | 0.52          |
| (2,1386) | 2:204:B:THR:HB   | 2:205:B:TRP:H    | 20       | 0.52          |
| (2,1334) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HG3  | 8        | 0.52          |
| (2,1251) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HG   | 1        | 0.52          |
| (2,1212) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HD2  | 1        | 0.52          |
| (2,619)  | 1:72:A:ILE:HB    | 2:216:B:ILE:HB   | 15       | 0.52          |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD11 | 15       | 0.52          |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD12 | 15       | 0.52          |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD13 | 15       | 0.52          |
| (1,12)   | 1:50:A:ARG:O     | 1:54:A:ILE:H     | 9        | 0.52          |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 8        | 0.52          |
| (2,2202) | 2:215:B:LYS:HB2  | 2:215:B:LYS:HE2  | 17       | 0.51          |
| (2,2202) | 2:215:B:LYS:HB2  | 2:215:B:LYS:HE3  | 17       | 0.51          |
| (2,2172) | 2:210:B:SER:HB2  | 2:215:B:LYS:HD2  | 2        | 0.51          |
| (2,2172) | 2:210:B:SER:HB3  | 2:215:B:LYS:HD2  | 2        | 0.51          |
| (2,2169) | 2:210:B:SER:HB2  | 2:212:B:ASN:H    | 6        | 0.51          |
| (2,2169) | 2:210:B:SER:HB3  | 2:212:B:ASN:H    | 6        | 0.51          |
| (2,2150) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG3  | 12       | 0.51          |
| (2,2150) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG3  | 12       | 0.51          |
| (2,2127) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HG   | 15       | 0.51          |
| (2,2127) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HG   | 15       | 0.51          |
| (2,2127) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HG   | 15       | 0.51          |
| (2,2127) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HG   | 15       | 0.51          |
| (2,2127) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HG   | 15       | 0.51          |
| (2,2127) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HG   | 15       | 0.51          |
| (2,1737) | 1:48:A:LEU:HD11  | 2:205:B:TRP:HZ2  | 6        | 0.51          |
| (2,1737) | 1:48:A:LEU:HD12  | 2:205:B:TRP:HZ2  | 6        | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1737) | 1:48:A:LEU:HD13  | 2:205:B:TRP:HZ2  | 6        | 0.51          |
| (2,1737) | 1:48:A:LEU:HD21  | 2:205:B:TRP:HZ2  | 6        | 0.51          |
| (2,1737) | 1:48:A:LEU:HD22  | 2:205:B:TRP:HZ2  | 6        | 0.51          |
| (2,1737) | 1:48:A:LEU:HD23  | 2:205:B:TRP:HZ2  | 6        | 0.51          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 19       | 0.51          |
| (2,1288) | 1:52:A:VAL:HG21  | 2:218:B:LEU:HG   | 11       | 0.51          |
| (2,1288) | 1:52:A:VAL:HG22  | 2:218:B:LEU:HG   | 11       | 0.51          |
| (2,1288) | 1:52:A:VAL:HG23  | 2:218:B:LEU:HG   | 11       | 0.51          |
| (2,991)  | 1:70:A:ILE:H     | 2:205:B:TRP:HZ3  | 6        | 0.51          |
| (2,616)  | 1:75:A:GLU:HA    | 2:214:B:LEU:HG   | 14       | 0.51          |
| (2,2112) | 2:206:B:ARG:HD2  | 2:207:B:VAL:H    | 7        | 0.5           |
| (2,2112) | 2:206:B:ARG:HD3  | 2:207:B:VAL:H    | 7        | 0.5           |
| (2,1737) | 1:48:A:LEU:HD11  | 2:205:B:TRP:HZ2  | 3        | 0.5           |
| (2,1737) | 1:48:A:LEU:HD12  | 2:205:B:TRP:HZ2  | 3        | 0.5           |
| (2,1737) | 1:48:A:LEU:HD13  | 2:205:B:TRP:HZ2  | 3        | 0.5           |
| (2,1737) | 1:48:A:LEU:HD21  | 2:205:B:TRP:HZ2  | 3        | 0.5           |
| (2,1737) | 1:48:A:LEU:HD22  | 2:205:B:TRP:HZ2  | 3        | 0.5           |
| (2,1737) | 1:48:A:LEU:HD23  | 2:205:B:TRP:HZ2  | 3        | 0.5           |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB2  | 3        | 0.5           |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB3  | 3        | 0.5           |
| (2,1489) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE3  | 9        | 0.5           |
| (2,1438) | 2:203:B:LEU:HD11 | 2:204:B:THR:H    | 9        | 0.5           |
| (2,1438) | 2:203:B:LEU:HD12 | 2:204:B:THR:H    | 9        | 0.5           |
| (2,1438) | 2:203:B:LEU:HD13 | 2:204:B:THR:H    | 9        | 0.5           |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H    | 9        | 0.5           |
| (2,1344) | 2:206:B:ARG:H    | 2:221:B:GLU:H    | 12       | 0.5           |
| (2,1333) | 1:34:A:ARG:HG2   | 2:213:B:PRO:HG3  | 15       | 0.5           |
| (2,1286) | 1:74:A:PHE:H     | 2:215:B:LYS:HG3  | 17       | 0.5           |
| (2,1253) | 2:214:B:LEU:HG   | 2:215:B:LYS:H    | 8        | 0.5           |
| (2,1252) | 2:214:B:LEU:H    | 2:214:B:LEU:HG   | 9        | 0.5           |
| (2,1237) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB2  | 17       | 0.5           |
| (2,1145) | 2:205:B:TRP:HE3  | 2:219:B:THR:HA   | 6        | 0.5           |
| (2,189)  | 1:70:A:ILE:HG12  | 2:205:B:TRP:HH2  | 11       | 0.5           |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 20       | 0.5           |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H     | 4        | 0.5           |
| (1,6)    | 1:35:A:GLN:O     | 1:39:A:ASP:H     | 1        | 0.5           |
| (2,2202) | 2:215:B:LYS:HB2  | 2:215:B:LYS:HE2  | 18       | 0.49          |
| (2,2202) | 2:215:B:LYS:HB2  | 2:215:B:LYS:HE3  | 18       | 0.49          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD11 | 14       | 0.49          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD12 | 14       | 0.49          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD13 | 14       | 0.49          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD21 | 14       | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD22 | 14       | 0.49          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD23 | 14       | 0.49          |
| (2,2112) | 2:206:B:ARG:HD2  | 2:207:B:VAL:H    | 11       | 0.49          |
| (2,2112) | 2:206:B:ARG:HD3  | 2:207:B:VAL:H    | 11       | 0.49          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD11 | 4        | 0.49          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD12 | 4        | 0.49          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD13 | 4        | 0.49          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD21 | 4        | 0.49          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD22 | 4        | 0.49          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD23 | 4        | 0.49          |
| (2,1407) | 2:213:B:PRO:HG2  | 2:214:B:LEU:H    | 3        | 0.49          |
| (2,1407) | 2:213:B:PRO:HG2  | 2:214:B:LEU:H    | 13       | 0.49          |
| (2,1386) | 2:204:B:THR:HB   | 2:205:B:TRP:H    | 9        | 0.49          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 5        | 0.49          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 14       | 0.49          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 15       | 0.49          |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H    | 18       | 0.49          |
| (2,1353) | 1:74:A:PHE:HD1   | 2:215:B:LYS:H    | 17       | 0.49          |
| (2,1353) | 1:74:A:PHE:HD2   | 2:215:B:LYS:H    | 17       | 0.49          |
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 13       | 0.49          |
| (2,1263) | 2:208:B:GLN:HE21 | 2:219:B:THR:HA   | 20       | 0.49          |
| (2,1145) | 2:205:B:TRP:HE3  | 2:219:B:THR:HA   | 12       | 0.49          |
| (2,531)  | 1:76:A:THR:HG21  | 2:215:B:LYS:HD3  | 14       | 0.49          |
| (2,531)  | 1:76:A:THR:HG22  | 2:215:B:LYS:HD3  | 14       | 0.49          |
| (2,531)  | 1:76:A:THR:HG23  | 2:215:B:LYS:HD3  | 14       | 0.49          |
| (2,16)   | 2:205:B:TRP:HZ3  | 2:218:B:LEU:HB3  | 2        | 0.49          |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 16       | 0.49          |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H     | 9        | 0.49          |
| (2,2208) | 2:216:B:ILE:HD11 | 2:218:B:LEU:HD11 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD11 | 2:218:B:LEU:HD12 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD11 | 2:218:B:LEU:HD13 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD11 | 2:218:B:LEU:HD21 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD11 | 2:218:B:LEU:HD22 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD11 | 2:218:B:LEU:HD23 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD12 | 2:218:B:LEU:HD11 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD12 | 2:218:B:LEU:HD12 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD12 | 2:218:B:LEU:HD13 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD12 | 2:218:B:LEU:HD21 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD12 | 2:218:B:LEU:HD22 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD12 | 2:218:B:LEU:HD23 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD13 | 2:218:B:LEU:HD11 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD13 | 2:218:B:LEU:HD12 | 18       | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2208) | 2:216:B:ILE:HD13 | 2:218:B:LEU:HD13 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD13 | 2:218:B:LEU:HD21 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD13 | 2:218:B:LEU:HD22 | 18       | 0.48          |
| (2,2208) | 2:216:B:ILE:HD13 | 2:218:B:LEU:HD23 | 18       | 0.48          |
| (2,2187) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE2  | 11       | 0.48          |
| (2,2187) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE3  | 11       | 0.48          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD11 | 18       | 0.48          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD12 | 18       | 0.48          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD13 | 18       | 0.48          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD21 | 18       | 0.48          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD22 | 18       | 0.48          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD23 | 18       | 0.48          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD11 | 5        | 0.48          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD12 | 5        | 0.48          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD13 | 5        | 0.48          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD21 | 5        | 0.48          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD22 | 5        | 0.48          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD23 | 5        | 0.48          |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD11 | 5        | 0.48          |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD12 | 5        | 0.48          |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD13 | 5        | 0.48          |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD21 | 5        | 0.48          |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD22 | 5        | 0.48          |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD23 | 5        | 0.48          |
| (2,1909) | 1:69:A:GLU:HG2   | 2:219:B:THR:HB   | 7        | 0.48          |
| (2,1909) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 7        | 0.48          |
| (2,1691) | 1:41:A:ASN:HD21  | 2:207:B:VAL:HB   | 16       | 0.48          |
| (2,1691) | 1:41:A:ASN:HD22  | 2:207:B:VAL:HB   | 16       | 0.48          |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 16       | 0.48          |
| (2,1407) | 2:213:B:PRO:HG2  | 2:214:B:LEU:H    | 8        | 0.48          |
| (2,1319) | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD21 | 17       | 0.48          |
| (2,1319) | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD22 | 17       | 0.48          |
| (2,1319) | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD23 | 17       | 0.48          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 5        | 0.48          |
| (2,1263) | 2:208:B:GLN:HE21 | 2:219:B:THR:HA   | 2        | 0.48          |
| (2,1152) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HA   | 9        | 0.48          |
| (2,1152) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HA   | 9        | 0.48          |
| (2,965)  | 1:74:A:PHE:H     | 2:214:B:LEU:HA   | 15       | 0.48          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 6        | 0.48          |
| (2,2216) | 2:217:B:ARG:HD2  | 2:219:B:THR:HB   | 16       | 0.47          |
| (2,2216) | 2:217:B:ARG:HD3  | 2:219:B:THR:HB   | 16       | 0.47          |
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE2  | 12       | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2188) | 2:212:B:ASN:HD22 | 2:215:B:LYS:HE3  | 12       | 0.47          |
| (2,2172) | 2:210:B:SER:HB2  | 2:215:B:LYS:HD2  | 4        | 0.47          |
| (2,2172) | 2:210:B:SER:HB3  | 2:215:B:LYS:HD2  | 4        | 0.47          |
| (2,2153) | 2:208:B:GLN:HG2  | 2:219:B:THR:HG21 | 2        | 0.47          |
| (2,2153) | 2:208:B:GLN:HG2  | 2:219:B:THR:HG22 | 2        | 0.47          |
| (2,2153) | 2:208:B:GLN:HG2  | 2:219:B:THR:HG23 | 2        | 0.47          |
| (2,2153) | 2:208:B:GLN:HG3  | 2:219:B:THR:HG21 | 2        | 0.47          |
| (2,2153) | 2:208:B:GLN:HG3  | 2:219:B:THR:HG22 | 2        | 0.47          |
| (2,2153) | 2:208:B:GLN:HG3  | 2:219:B:THR:HG23 | 2        | 0.47          |
| (2,1910) | 1:69:A:GLU:HG2   | 2:219:B:THR:HG21 | 11       | 0.47          |
| (2,1910) | 1:69:A:GLU:HG2   | 2:219:B:THR:HG22 | 11       | 0.47          |
| (2,1910) | 1:69:A:GLU:HG2   | 2:219:B:THR:HG23 | 11       | 0.47          |
| (2,1910) | 1:69:A:GLU:HG3   | 2:219:B:THR:HG21 | 11       | 0.47          |
| (2,1910) | 1:69:A:GLU:HG3   | 2:219:B:THR:HG22 | 11       | 0.47          |
| (2,1910) | 1:69:A:GLU:HG3   | 2:219:B:THR:HG23 | 11       | 0.47          |
| (2,1794) | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ3  | 15       | 0.47          |
| (2,1794) | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ3  | 15       | 0.47          |
| (2,1794) | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ3  | 15       | 0.47          |
| (2,1794) | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ3  | 15       | 0.47          |
| (2,1794) | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ3  | 15       | 0.47          |
| (2,1794) | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ3  | 15       | 0.47          |
| (2,1794) | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ3  | 17       | 0.47          |
| (2,1794) | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ3  | 17       | 0.47          |
| (2,1794) | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ3  | 17       | 0.47          |
| (2,1794) | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ3  | 17       | 0.47          |
| (2,1794) | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ3  | 17       | 0.47          |
| (2,1794) | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ3  | 17       | 0.47          |
| (2,1605) | 1:34:A:ARG:HD2   | 2:213:B:PRO:HB2  | 17       | 0.47          |
| (2,1605) | 1:34:A:ARG:HD2   | 2:213:B:PRO:HB3  | 17       | 0.47          |
| (2,1605) | 1:34:A:ARG:HD3   | 2:213:B:PRO:HB2  | 17       | 0.47          |
| (2,1605) | 1:34:A:ARG:HD3   | 2:213:B:PRO:HB3  | 17       | 0.47          |
| (2,1393) | 2:206:B:ARG:H    | 2:206:B:ARG:HD2  | 2        | 0.47          |
| (2,1386) | 2:204:B:THR:HB   | 2:205:B:TRP:H    | 17       | 0.47          |
| (2,1273) | 2:220:B:ARG:HD3  | 2:221:B:GLU:H    | 18       | 0.47          |
| (2,1202) | 2:215:B:LYS:HG2  | 2:216:B:ILE:H    | 20       | 0.47          |
| (2,58)   | 1:76:A:THR:HG21  | 2:215:B:LYS:HG3  | 4        | 0.47          |
| (2,58)   | 1:76:A:THR:HG22  | 2:215:B:LYS:HG3  | 4        | 0.47          |
| (2,58)   | 1:76:A:THR:HG23  | 2:215:B:LYS:HG3  | 4        | 0.47          |
| (2,47)   | 1:72:A:ILE:HA    | 2:216:B:ILE:HD11 | 15       | 0.47          |
| (2,47)   | 1:72:A:ILE:HA    | 2:216:B:ILE:HD12 | 15       | 0.47          |
| (2,47)   | 1:72:A:ILE:HA    | 2:216:B:ILE:HD13 | 15       | 0.47          |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H     | 16       | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD11 | 1        | 0.46          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD12 | 1        | 0.46          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD13 | 1        | 0.46          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD21 | 1        | 0.46          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD22 | 1        | 0.46          |
| (2,2193) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD23 | 1        | 0.46          |
| (2,2182) | 2:212:B:ASN:HB2  | 2:214:B:LEU:HD11 | 20       | 0.46          |
| (2,2182) | 2:212:B:ASN:HB2  | 2:214:B:LEU:HD12 | 20       | 0.46          |
| (2,2182) | 2:212:B:ASN:HB2  | 2:214:B:LEU:HD13 | 20       | 0.46          |
| (2,2182) | 2:212:B:ASN:HB2  | 2:214:B:LEU:HD21 | 20       | 0.46          |
| (2,2182) | 2:212:B:ASN:HB2  | 2:214:B:LEU:HD22 | 20       | 0.46          |
| (2,2182) | 2:212:B:ASN:HB2  | 2:214:B:LEU:HD23 | 20       | 0.46          |
| (2,2182) | 2:212:B:ASN:HB3  | 2:214:B:LEU:HD11 | 20       | 0.46          |
| (2,2182) | 2:212:B:ASN:HB3  | 2:214:B:LEU:HD12 | 20       | 0.46          |
| (2,2182) | 2:212:B:ASN:HB3  | 2:214:B:LEU:HD13 | 20       | 0.46          |
| (2,2182) | 2:212:B:ASN:HB3  | 2:214:B:LEU:HD21 | 20       | 0.46          |
| (2,2182) | 2:212:B:ASN:HB3  | 2:214:B:LEU:HD22 | 20       | 0.46          |
| (2,2182) | 2:212:B:ASN:HB3  | 2:214:B:LEU:HD23 | 20       | 0.46          |
| (2,2165) | 2:209:B:ARG:HD2  | 2:210:B:SER:H    | 1        | 0.46          |
| (2,2165) | 2:209:B:ARG:HD3  | 2:210:B:SER:H    | 1        | 0.46          |
| (2,2127) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HG   | 5        | 0.46          |
| (2,2127) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HG   | 5        | 0.46          |
| (2,2127) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HG   | 5        | 0.46          |
| (2,2127) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HG   | 5        | 0.46          |
| (2,2127) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HG   | 5        | 0.46          |
| (2,2127) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HG   | 5        | 0.46          |
| (2,2122) | 2:207:B:VAL:HG11 | 2:217:B:ARG:H    | 18       | 0.46          |
| (2,2122) | 2:207:B:VAL:HG12 | 2:217:B:ARG:H    | 18       | 0.46          |
| (2,2122) | 2:207:B:VAL:HG13 | 2:217:B:ARG:H    | 18       | 0.46          |
| (2,2122) | 2:207:B:VAL:HG21 | 2:217:B:ARG:H    | 18       | 0.46          |
| (2,2122) | 2:207:B:VAL:HG22 | 2:217:B:ARG:H    | 18       | 0.46          |
| (2,2122) | 2:207:B:VAL:HG23 | 2:217:B:ARG:H    | 18       | 0.46          |
| (2,2118) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD11 | 9        | 0.46          |
| (2,2118) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD12 | 9        | 0.46          |
| (2,2118) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD13 | 9        | 0.46          |
| (2,2118) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD21 | 9        | 0.46          |
| (2,2118) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD22 | 9        | 0.46          |
| (2,2118) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD23 | 9        | 0.46          |
| (2,1438) | 2:203:B:LEU:HD11 | 2:204:B:THR:H    | 17       | 0.46          |
| (2,1438) | 2:203:B:LEU:HD12 | 2:204:B:THR:H    | 17       | 0.46          |
| (2,1438) | 2:203:B:LEU:HD13 | 2:204:B:THR:H    | 17       | 0.46          |
| (2,1396) | 2:205:B:TRP:HB2  | 2:206:B:ARG:H    | 16       | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1204) | 1:73:A:ASP:HA    | 2:215:B:LYS:HG2  | 2        | 0.46          |
| (2,100)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HH2  | 19       | 0.46          |
| (2,100)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HH2  | 19       | 0.46          |
| (2,100)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HH2  | 19       | 0.46          |
| (1,21)   | 1:87:A:ARG:O     | 1:91:A:SER:N     | 12       | 0.46          |
| (1,17)   | 1:53:A:HIS:O     | 1:57:A:SER:N     | 11       | 0.46          |
| (2,2177) | 2:212:B:ASN:H    | 2:215:B:LYS:HE2  | 10       | 0.45          |
| (2,2177) | 2:212:B:ASN:H    | 2:215:B:LYS:HE3  | 10       | 0.45          |
| (2,2122) | 2:207:B:VAL:HG11 | 2:217:B:ARG:H    | 1        | 0.45          |
| (2,2122) | 2:207:B:VAL:HG12 | 2:217:B:ARG:H    | 1        | 0.45          |
| (2,2122) | 2:207:B:VAL:HG13 | 2:217:B:ARG:H    | 1        | 0.45          |
| (2,2122) | 2:207:B:VAL:HG21 | 2:217:B:ARG:H    | 1        | 0.45          |
| (2,2122) | 2:207:B:VAL:HG22 | 2:217:B:ARG:H    | 1        | 0.45          |
| (2,2122) | 2:207:B:VAL:HG23 | 2:217:B:ARG:H    | 1        | 0.45          |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD11 | 2        | 0.45          |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD12 | 2        | 0.45          |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD13 | 2        | 0.45          |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD21 | 2        | 0.45          |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD22 | 2        | 0.45          |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD23 | 2        | 0.45          |
| (2,1475) | 1:73:A:ASP:HA    | 2:216:B:ILE:H    | 20       | 0.45          |
| (2,1471) | 1:74:A:PHE:H     | 2:215:B:LYS:H    | 9        | 0.45          |
| (2,1386) | 2:204:B:THR:HB   | 2:205:B:TRP:H    | 1        | 0.45          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 11       | 0.45          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 15       | 0.45          |
| (2,1250) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HG   | 1        | 0.45          |
| (2,1250) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HG   | 1        | 0.45          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 10       | 0.45          |
| (1,13)   | 1:51:A:VAL:O     | 1:55:A:ILE:N     | 5        | 0.45          |
| (1,12)   | 1:50:A:ARG:O     | 1:54:A:ILE:H     | 18       | 0.45          |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD2  | 18       | 0.44          |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD3  | 18       | 0.44          |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD2  | 18       | 0.44          |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD3  | 18       | 0.44          |
| (2,1740) | 1:48:A:LEU:HD11  | 2:206:B:ARG:HB2  | 2        | 0.44          |
| (2,1740) | 1:48:A:LEU:HD11  | 2:206:B:ARG:HB3  | 2        | 0.44          |
| (2,1740) | 1:48:A:LEU:HD12  | 2:206:B:ARG:HB2  | 2        | 0.44          |
| (2,1740) | 1:48:A:LEU:HD12  | 2:206:B:ARG:HB3  | 2        | 0.44          |
| (2,1740) | 1:48:A:LEU:HD13  | 2:206:B:ARG:HB2  | 2        | 0.44          |
| (2,1740) | 1:48:A:LEU:HD13  | 2:206:B:ARG:HB3  | 2        | 0.44          |
| (2,1740) | 1:48:A:LEU:HD21  | 2:206:B:ARG:HB2  | 2        | 0.44          |
| (2,1740) | 1:48:A:LEU:HD21  | 2:206:B:ARG:HB3  | 2        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1740) | 1:48:A:LEU:HD22  | 2:206:B:ARG:HB2  | 2        | 0.44          |
| (2,1740) | 1:48:A:LEU:HD22  | 2:206:B:ARG:HB3  | 2        | 0.44          |
| (2,1740) | 1:48:A:LEU:HD23  | 2:206:B:ARG:HB2  | 2        | 0.44          |
| (2,1740) | 1:48:A:LEU:HD23  | 2:206:B:ARG:HB3  | 2        | 0.44          |
| (2,1471) | 1:74:A:PHE:H     | 2:215:B:LYS:H    | 13       | 0.44          |
| (2,1455) | 1:74:A:PHE:H     | 2:214:B:LEU:H    | 14       | 0.44          |
| (2,1403) | 2:221:B:GLU:HB3  | 2:222:B:ALA:H    | 11       | 0.44          |
| (2,1403) | 2:221:B:GLU:HB3  | 2:222:B:ALA:H    | 17       | 0.44          |
| (2,1392) | 2:209:B:ARG:HD3  | 2:210:B:SER:H    | 1        | 0.44          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 16       | 0.44          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD11 | 14       | 0.44          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD12 | 14       | 0.44          |
| (2,1335) | 2:213:B:PRO:HG3  | 2:214:B:LEU:HD13 | 14       | 0.44          |
| (2,1224) | 1:70:A:ILE:HD11  | 2:219:B:THR:HA   | 11       | 0.44          |
| (2,1224) | 1:70:A:ILE:HD12  | 2:219:B:THR:HA   | 11       | 0.44          |
| (2,1224) | 1:70:A:ILE:HD13  | 2:219:B:THR:HA   | 11       | 0.44          |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD11 | 11       | 0.44          |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD12 | 11       | 0.44          |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD13 | 11       | 0.44          |
| (2,1190) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD21 | 18       | 0.44          |
| (2,1190) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD22 | 18       | 0.44          |
| (2,1190) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD23 | 18       | 0.44          |
| (2,1187) | 2:217:B:ARG:HG2  | 2:218:B:LEU:H    | 12       | 0.44          |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 7        | 0.44          |
| (2,2105) | 2:206:B:ARG:HB2  | 2:207:B:VAL:H    | 2        | 0.43          |
| (2,2105) | 2:206:B:ARG:HB3  | 2:207:B:VAL:H    | 2        | 0.43          |
| (2,1737) | 1:48:A:LEU:HD11  | 2:205:B:TRP:HZ2  | 8        | 0.43          |
| (2,1737) | 1:48:A:LEU:HD12  | 2:205:B:TRP:HZ2  | 8        | 0.43          |
| (2,1737) | 1:48:A:LEU:HD13  | 2:205:B:TRP:HZ2  | 8        | 0.43          |
| (2,1737) | 1:48:A:LEU:HD21  | 2:205:B:TRP:HZ2  | 8        | 0.43          |
| (2,1737) | 1:48:A:LEU:HD22  | 2:205:B:TRP:HZ2  | 8        | 0.43          |
| (2,1737) | 1:48:A:LEU:HD23  | 2:205:B:TRP:HZ2  | 8        | 0.43          |
| (2,1625) | 1:36:A:LEU:H     | 2:214:B:LEU:HD11 | 4        | 0.43          |
| (2,1625) | 1:36:A:LEU:H     | 2:214:B:LEU:HD12 | 4        | 0.43          |
| (2,1625) | 1:36:A:LEU:H     | 2:214:B:LEU:HD13 | 4        | 0.43          |
| (2,1625) | 1:36:A:LEU:H     | 2:214:B:LEU:HD21 | 4        | 0.43          |
| (2,1625) | 1:36:A:LEU:H     | 2:214:B:LEU:HD22 | 4        | 0.43          |
| (2,1625) | 1:36:A:LEU:H     | 2:214:B:LEU:HD23 | 4        | 0.43          |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 13       | 0.43          |
| (2,1386) | 2:204:B:THR:HB   | 2:205:B:TRP:H    | 13       | 0.43          |
| (2,1242) | 1:70:A:ILE:H     | 2:219:B:THR:HA   | 15       | 0.43          |
| (2,1233) | 2:204:B:THR:HG21 | 2:205:B:TRP:HB3  | 8        | 0.43          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1233) | 2:204:B:THR:HG22 | 2:205:B:TRP:HB3 | 8        | 0.43          |
| (2,1233) | 2:204:B:THR:HG23 | 2:205:B:TRP:HB3 | 8        | 0.43          |
| (2,1233) | 2:204:B:THR:HG21 | 2:205:B:TRP:HB3 | 20       | 0.43          |
| (2,1233) | 2:204:B:THR:HG22 | 2:205:B:TRP:HB3 | 20       | 0.43          |
| (2,1233) | 2:204:B:THR:HG23 | 2:205:B:TRP:HB3 | 20       | 0.43          |
| (2,1231) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HA  | 5        | 0.43          |
| (2,965)  | 1:74:A:PHE:H     | 2:214:B:LEU:HA  | 9        | 0.43          |
| (2,28)   | 1:69:A:GLU:HA    | 2:205:B:TRP:HZ3 | 7        | 0.43          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1 | 1        | 0.43          |
| (2,2199) | 2:214:B:LEU:HD11 | 2:215:B:LYS:H   | 1        | 0.42          |
| (2,2199) | 2:214:B:LEU:HD12 | 2:215:B:LYS:H   | 1        | 0.42          |
| (2,2199) | 2:214:B:LEU:HD13 | 2:215:B:LYS:H   | 1        | 0.42          |
| (2,2199) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H   | 1        | 0.42          |
| (2,2199) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H   | 1        | 0.42          |
| (2,2199) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H   | 1        | 0.42          |
| (2,2154) | 2:208:B:GLN:HE22 | 2:217:B:ARG:HD2 | 6        | 0.42          |
| (2,2154) | 2:208:B:GLN:HE22 | 2:217:B:ARG:HD3 | 6        | 0.42          |
| (2,2150) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG3 | 7        | 0.42          |
| (2,2150) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG3 | 7        | 0.42          |
| (2,2148) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HB3 | 15       | 0.42          |
| (2,2148) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HB3 | 15       | 0.42          |
| (2,2140) | 2:208:B:GLN:HB2  | 2:217:B:ARG:HD2 | 13       | 0.42          |
| (2,2140) | 2:208:B:GLN:HB2  | 2:217:B:ARG:HD3 | 13       | 0.42          |
| (2,2140) | 2:208:B:GLN:HB3  | 2:217:B:ARG:HD2 | 13       | 0.42          |
| (2,2140) | 2:208:B:GLN:HB3  | 2:217:B:ARG:HD3 | 13       | 0.42          |
| (2,1931) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG3 | 10       | 0.42          |
| (2,1931) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG3 | 10       | 0.42          |
| (2,1736) | 1:48:A:LEU:HD11  | 2:205:B:TRP:H   | 18       | 0.42          |
| (2,1736) | 1:48:A:LEU:HD12  | 2:205:B:TRP:H   | 18       | 0.42          |
| (2,1736) | 1:48:A:LEU:HD13  | 2:205:B:TRP:H   | 18       | 0.42          |
| (2,1736) | 1:48:A:LEU:HD21  | 2:205:B:TRP:H   | 18       | 0.42          |
| (2,1736) | 1:48:A:LEU:HD22  | 2:205:B:TRP:H   | 18       | 0.42          |
| (2,1736) | 1:48:A:LEU:HD23  | 2:205:B:TRP:H   | 18       | 0.42          |
| (2,1438) | 2:203:B:LEU:HD11 | 2:204:B:THR:H   | 12       | 0.42          |
| (2,1438) | 2:203:B:LEU:HD12 | 2:204:B:THR:H   | 12       | 0.42          |
| (2,1438) | 2:203:B:LEU:HD13 | 2:204:B:THR:H   | 12       | 0.42          |
| (2,1367) | 1:73:A:ASP:HA    | 2:215:B:LYS:H   | 15       | 0.42          |
| (2,1294) | 2:204:B:THR:HG21 | 2:205:B:TRP:HD1 | 4        | 0.42          |
| (2,1294) | 2:204:B:THR:HG22 | 2:205:B:TRP:HD1 | 4        | 0.42          |
| (2,1294) | 2:204:B:THR:HG23 | 2:205:B:TRP:HD1 | 4        | 0.42          |
| (2,1272) | 1:69:A:GLU:HG2   | 2:219:B:THR:HB  | 9        | 0.42          |
| (2,1127) | 1:70:A:ILE:H     | 2:205:B:TRP:HH2 | 6        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,531)  | 1:76:A:THR:HG21  | 2:215:B:LYS:HD3  | 15       | 0.42          |
| (2,531)  | 1:76:A:THR:HG22  | 2:215:B:LYS:HD3  | 15       | 0.42          |
| (2,531)  | 1:76:A:THR:HG23  | 2:215:B:LYS:HD3  | 15       | 0.42          |
| (2,30)   | 1:30:A:TYR:HE1   | 2:214:B:LEU:HG   | 10       | 0.42          |
| (2,30)   | 1:30:A:TYR:HE2   | 2:214:B:LEU:HG   | 10       | 0.42          |
| (1,18)   | 1:53:A:HIS:O     | 1:57:A:SER:H     | 11       | 0.42          |
| (1,12)   | 1:50:A:ARG:O     | 1:54:A:ILE:H     | 8        | 0.42          |
| (1,9)    | 1:49:A:GLY:O     | 1:53:A:HIS:N     | 11       | 0.42          |
| (2,2203) | 2:215:B:LYS:HB3  | 2:215:B:LYS:HE2  | 18       | 0.41          |
| (2,2203) | 2:215:B:LYS:HB3  | 2:215:B:LYS:HE3  | 18       | 0.41          |
| (2,2149) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HG2  | 12       | 0.41          |
| (2,2149) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HG2  | 12       | 0.41          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD11 | 7        | 0.41          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD12 | 7        | 0.41          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD13 | 7        | 0.41          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD21 | 7        | 0.41          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD22 | 7        | 0.41          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD23 | 7        | 0.41          |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 7        | 0.41          |
| (2,1479) | 2:208:B:GLN:HE21 | 2:219:B:THR:HB   | 4        | 0.41          |
| (2,1340) | 2:205:B:TRP:HE3  | 2:219:B:THR:H    | 9        | 0.41          |
| (2,1261) | 2:214:B:LEU:HA   | 2:215:B:LYS:HB2  | 2        | 0.41          |
| (2,1227) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HA   | 14       | 0.41          |
| (2,1224) | 1:70:A:ILE:HD11  | 2:219:B:THR:HA   | 5        | 0.41          |
| (2,1224) | 1:70:A:ILE:HD12  | 2:219:B:THR:HA   | 5        | 0.41          |
| (2,1224) | 1:70:A:ILE:HD13  | 2:219:B:THR:HA   | 5        | 0.41          |
| (2,176)  | 1:73:A:ASP:HA    | 2:215:B:LYS:HD3  | 12       | 0.41          |
| (1,13)   | 1:51:A:VAL:O     | 1:55:A:ILE:N     | 7        | 0.41          |
| (2,2203) | 2:215:B:LYS:HB3  | 2:215:B:LYS:HE2  | 17       | 0.4           |
| (2,2203) | 2:215:B:LYS:HB3  | 2:215:B:LYS:HE3  | 17       | 0.4           |
| (2,2169) | 2:210:B:SER:HB2  | 2:212:B:ASN:H    | 2        | 0.4           |
| (2,2169) | 2:210:B:SER:HB3  | 2:212:B:ASN:H    | 2        | 0.4           |
| (2,2140) | 2:208:B:GLN:HB2  | 2:217:B:ARG:HD2  | 17       | 0.4           |
| (2,2140) | 2:208:B:GLN:HB2  | 2:217:B:ARG:HD3  | 17       | 0.4           |
| (2,2140) | 2:208:B:GLN:HB3  | 2:217:B:ARG:HD2  | 17       | 0.4           |
| (2,2140) | 2:208:B:GLN:HB3  | 2:217:B:ARG:HD3  | 17       | 0.4           |
| (2,2118) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD11 | 14       | 0.4           |
| (2,2118) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD12 | 14       | 0.4           |
| (2,2118) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD13 | 14       | 0.4           |
| (2,2118) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD21 | 14       | 0.4           |
| (2,2118) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD22 | 14       | 0.4           |
| (2,2118) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD23 | 14       | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD11 | 6        | 0.4           |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD12 | 6        | 0.4           |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD13 | 6        | 0.4           |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD21 | 6        | 0.4           |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD22 | 6        | 0.4           |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD23 | 6        | 0.4           |
| (2,1909) | 1:69:A:GLU:HG2   | 2:219:B:THR:HB   | 1        | 0.4           |
| (2,1909) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 1        | 0.4           |
| (2,1903) | 1:68:A:ASP:HB3   | 2:220:B:ARG:HG2  | 17       | 0.4           |
| (2,1903) | 1:68:A:ASP:HB3   | 2:220:B:ARG:HG3  | 17       | 0.4           |
| (2,1795) | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ2  | 3        | 0.4           |
| (2,1795) | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ2  | 3        | 0.4           |
| (2,1795) | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ2  | 3        | 0.4           |
| (2,1795) | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ2  | 3        | 0.4           |
| (2,1795) | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ2  | 3        | 0.4           |
| (2,1795) | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ2  | 3        | 0.4           |
| (2,1233) | 2:204:B:THR:HG21 | 2:205:B:TRP:HB3  | 16       | 0.4           |
| (2,1233) | 2:204:B:THR:HG22 | 2:205:B:TRP:HB3  | 16       | 0.4           |
| (2,1233) | 2:204:B:THR:HG23 | 2:205:B:TRP:HB3  | 16       | 0.4           |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD11 | 10       | 0.4           |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD12 | 10       | 0.4           |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD13 | 10       | 0.4           |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD11 | 13       | 0.4           |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD12 | 13       | 0.4           |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD13 | 13       | 0.4           |
| (2,1114) | 1:37:A:SER:H     | 2:214:B:LEU:HA   | 6        | 0.4           |
| (2,803)  | 1:75:A:GLU:H     | 2:214:B:LEU:HB2  | 15       | 0.4           |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 7        | 0.4           |
| (1,13)   | 1:51:A:VAL:O     | 1:55:A:ILE:N     | 15       | 0.4           |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 17       | 0.4           |
| (2,2199) | 2:214:B:LEU:HD11 | 2:215:B:LYS:H    | 20       | 0.39          |
| (2,2199) | 2:214:B:LEU:HD12 | 2:215:B:LYS:H    | 20       | 0.39          |
| (2,2199) | 2:214:B:LEU:HD13 | 2:215:B:LYS:H    | 20       | 0.39          |
| (2,2199) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H    | 20       | 0.39          |
| (2,2199) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H    | 20       | 0.39          |
| (2,2199) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H    | 20       | 0.39          |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD11 | 9        | 0.39          |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD12 | 9        | 0.39          |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD13 | 9        | 0.39          |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD21 | 9        | 0.39          |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD22 | 9        | 0.39          |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD23 | 9        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2184) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HB3  | 14       | 0.39          |
| (2,2184) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB3  | 14       | 0.39          |
| (2,1737) | 1:48:A:LEU:HD11  | 2:205:B:TRP:HZ2  | 11       | 0.39          |
| (2,1737) | 1:48:A:LEU:HD12  | 2:205:B:TRP:HZ2  | 11       | 0.39          |
| (2,1737) | 1:48:A:LEU:HD13  | 2:205:B:TRP:HZ2  | 11       | 0.39          |
| (2,1737) | 1:48:A:LEU:HD21  | 2:205:B:TRP:HZ2  | 11       | 0.39          |
| (2,1737) | 1:48:A:LEU:HD22  | 2:205:B:TRP:HZ2  | 11       | 0.39          |
| (2,1737) | 1:48:A:LEU:HD23  | 2:205:B:TRP:HZ2  | 11       | 0.39          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 2        | 0.39          |
| (2,1267) | 2:205:B:TRP:HE3  | 2:220:B:ARG:HB3  | 7        | 0.39          |
| (2,1265) | 2:204:B:THR:HB   | 2:205:B:TRP:HB3  | 6        | 0.39          |
| (2,1206) | 1:73:A:ASP:HA    | 2:215:B:LYS:HG3  | 17       | 0.39          |
| (2,1187) | 2:217:B:ARG:HG2  | 2:218:B:LEU:H    | 4        | 0.39          |
| (2,1152) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HA   | 13       | 0.39          |
| (2,1152) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HA   | 13       | 0.39          |
| (2,1104) | 1:73:A:ASP:H     | 2:215:B:LYS:HA   | 9        | 0.39          |
| (2,531)  | 1:76:A:THR:HG21  | 2:215:B:LYS:HD3  | 3        | 0.39          |
| (2,531)  | 1:76:A:THR:HG22  | 2:215:B:LYS:HD3  | 3        | 0.39          |
| (2,531)  | 1:76:A:THR:HG23  | 2:215:B:LYS:HD3  | 3        | 0.39          |
| (2,177)  | 1:73:A:ASP:HA    | 2:216:B:ILE:HG21 | 14       | 0.39          |
| (2,177)  | 1:73:A:ASP:HA    | 2:216:B:ILE:HG22 | 14       | 0.39          |
| (2,177)  | 1:73:A:ASP:HA    | 2:216:B:ILE:HG23 | 14       | 0.39          |
| (2,176)  | 1:73:A:ASP:HA    | 2:215:B:LYS:HD3  | 17       | 0.39          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 5        | 0.39          |
| (1,22)   | 1:87:A:ARG:O     | 1:91:A:SER:H     | 12       | 0.39          |
| (1,17)   | 1:53:A:HIS:O     | 1:57:A:SER:N     | 17       | 0.39          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 5        | 0.39          |
| (1,12)   | 1:50:A:ARG:O     | 1:54:A:ILE:H     | 16       | 0.39          |
| (1,9)    | 1:49:A:GLY:O     | 1:53:A:HIS:N     | 9        | 0.39          |
| (2,2222) | 2:218:B:LEU:HD11 | 2:219:B:THR:H    | 4        | 0.38          |
| (2,2222) | 2:218:B:LEU:HD12 | 2:219:B:THR:H    | 4        | 0.38          |
| (2,2222) | 2:218:B:LEU:HD13 | 2:219:B:THR:H    | 4        | 0.38          |
| (2,2222) | 2:218:B:LEU:HD21 | 2:219:B:THR:H    | 4        | 0.38          |
| (2,2222) | 2:218:B:LEU:HD22 | 2:219:B:THR:H    | 4        | 0.38          |
| (2,2222) | 2:218:B:LEU:HD23 | 2:219:B:THR:H    | 4        | 0.38          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD11 | 8        | 0.38          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD12 | 8        | 0.38          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD13 | 8        | 0.38          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD21 | 8        | 0.38          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD22 | 8        | 0.38          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD23 | 8        | 0.38          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD11 | 13       | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD12 | 13       | 0.38          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD13 | 13       | 0.38          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD21 | 13       | 0.38          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD22 | 13       | 0.38          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD23 | 13       | 0.38          |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD11 | 13       | 0.38          |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD12 | 13       | 0.38          |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD13 | 13       | 0.38          |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD21 | 13       | 0.38          |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD22 | 13       | 0.38          |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD23 | 13       | 0.38          |
| (2,1903) | 1:68:A:ASP:HB3   | 2:220:B:ARG:HG2  | 5        | 0.38          |
| (2,1903) | 1:68:A:ASP:HB3   | 2:220:B:ARG:HG3  | 5        | 0.38          |
| (2,1736) | 1:48:A:LEU:HD11  | 2:205:B:TRP:H    | 7        | 0.38          |
| (2,1736) | 1:48:A:LEU:HD12  | 2:205:B:TRP:H    | 7        | 0.38          |
| (2,1736) | 1:48:A:LEU:HD13  | 2:205:B:TRP:H    | 7        | 0.38          |
| (2,1736) | 1:48:A:LEU:HD21  | 2:205:B:TRP:H    | 7        | 0.38          |
| (2,1736) | 1:48:A:LEU:HD22  | 2:205:B:TRP:H    | 7        | 0.38          |
| (2,1736) | 1:48:A:LEU:HD23  | 2:205:B:TRP:H    | 7        | 0.38          |
| (2,1490) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE2  | 7        | 0.38          |
| (2,1461) | 2:212:B:ASN:H    | 2:215:B:LYS:HB2  | 10       | 0.38          |
| (2,1438) | 2:203:B:LEU:HD11 | 2:204:B:THR:H    | 18       | 0.38          |
| (2,1438) | 2:203:B:LEU:HD12 | 2:204:B:THR:H    | 18       | 0.38          |
| (2,1438) | 2:203:B:LEU:HD13 | 2:204:B:THR:H    | 18       | 0.38          |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG   | 9        | 0.38          |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG   | 19       | 0.38          |
| (2,1393) | 2:206:B:ARG:H    | 2:206:B:ARG:HD2  | 11       | 0.38          |
| (2,1355) | 1:74:A:PHE:HD1   | 2:214:B:LEU:H    | 9        | 0.38          |
| (2,1355) | 1:74:A:PHE:HD2   | 2:214:B:LEU:H    | 9        | 0.38          |
| (2,1232) | 2:218:B:LEU:HA   | 2:219:B:THR:HG21 | 7        | 0.38          |
| (2,1232) | 2:218:B:LEU:HA   | 2:219:B:THR:HG22 | 7        | 0.38          |
| (2,1232) | 2:218:B:LEU:HA   | 2:219:B:THR:HG23 | 7        | 0.38          |
| (2,1162) | 1:68:A:ASP:HB2   | 2:220:B:ARG:HB3  | 1        | 0.38          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 15       | 0.38          |
| (2,2222) | 2:218:B:LEU:HD11 | 2:219:B:THR:H    | 16       | 0.37          |
| (2,2222) | 2:218:B:LEU:HD12 | 2:219:B:THR:H    | 16       | 0.37          |
| (2,2222) | 2:218:B:LEU:HD13 | 2:219:B:THR:H    | 16       | 0.37          |
| (2,2222) | 2:218:B:LEU:HD21 | 2:219:B:THR:H    | 16       | 0.37          |
| (2,2222) | 2:218:B:LEU:HD22 | 2:219:B:THR:H    | 16       | 0.37          |
| (2,2222) | 2:218:B:LEU:HD23 | 2:219:B:THR:H    | 16       | 0.37          |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD11 | 6        | 0.37          |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD12 | 6        | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD13 | 6        | 0.37          |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD21 | 6        | 0.37          |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD22 | 6        | 0.37          |
| (2,2194) | 2:213:B:PRO:HD2  | 2:214:B:LEU:HD23 | 6        | 0.37          |
| (2,2122) | 2:207:B:VAL:HG11 | 2:217:B:ARG:H    | 20       | 0.37          |
| (2,2122) | 2:207:B:VAL:HG12 | 2:217:B:ARG:H    | 20       | 0.37          |
| (2,2122) | 2:207:B:VAL:HG13 | 2:217:B:ARG:H    | 20       | 0.37          |
| (2,2122) | 2:207:B:VAL:HG21 | 2:217:B:ARG:H    | 20       | 0.37          |
| (2,2122) | 2:207:B:VAL:HG22 | 2:217:B:ARG:H    | 20       | 0.37          |
| (2,2122) | 2:207:B:VAL:HG23 | 2:217:B:ARG:H    | 20       | 0.37          |
| (2,1930) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG2  | 20       | 0.37          |
| (2,1930) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG2  | 20       | 0.37          |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB2  | 19       | 0.37          |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB3  | 19       | 0.37          |
| (2,1459) | 2:220:B:ARG:HD2  | 2:221:B:GLU:H    | 18       | 0.37          |
| (2,1398) | 1:68:A:ASP:HB2   | 2:220:B:ARG:H    | 14       | 0.37          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 17       | 0.37          |
| (2,1294) | 2:204:B:THR:HG21 | 2:205:B:TRP:HD1  | 8        | 0.37          |
| (2,1294) | 2:204:B:THR:HG22 | 2:205:B:TRP:HD1  | 8        | 0.37          |
| (2,1294) | 2:204:B:THR:HG23 | 2:205:B:TRP:HD1  | 8        | 0.37          |
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 17       | 0.37          |
| (2,1242) | 1:70:A:ILE:H     | 2:219:B:THR:HA   | 11       | 0.37          |
| (2,1237) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB2  | 18       | 0.37          |
| (2,1171) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HB2  | 3        | 0.37          |
| (2,803)  | 1:75:A:GLU:H     | 2:214:B:LEU:HB2  | 14       | 0.37          |
| (2,176)  | 1:73:A:ASP:HA    | 2:215:B:LYS:HD3  | 18       | 0.37          |
| (2,162)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ3  | 19       | 0.37          |
| (2,162)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ3  | 19       | 0.37          |
| (2,162)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ3  | 19       | 0.37          |
| (2,2216) | 2:217:B:ARG:HD2  | 2:219:B:THR:HB   | 4        | 0.36          |
| (2,2216) | 2:217:B:ARG:HD3  | 2:219:B:THR:HB   | 4        | 0.36          |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD2  | 15       | 0.36          |
| (2,2151) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HD3  | 15       | 0.36          |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD2  | 15       | 0.36          |
| (2,2151) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HD3  | 15       | 0.36          |
| (2,2148) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HB3  | 8        | 0.36          |
| (2,2148) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HB3  | 8        | 0.36          |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD11 | 13       | 0.36          |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD12 | 13       | 0.36          |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD13 | 13       | 0.36          |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD21 | 13       | 0.36          |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD22 | 13       | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD23 | 13       | 0.36          |
| (2,1737) | 1:48:A:LEU:HD11  | 2:205:B:TRP:HZ2  | 12       | 0.36          |
| (2,1737) | 1:48:A:LEU:HD12  | 2:205:B:TRP:HZ2  | 12       | 0.36          |
| (2,1737) | 1:48:A:LEU:HD13  | 2:205:B:TRP:HZ2  | 12       | 0.36          |
| (2,1737) | 1:48:A:LEU:HD21  | 2:205:B:TRP:HZ2  | 12       | 0.36          |
| (2,1737) | 1:48:A:LEU:HD22  | 2:205:B:TRP:HZ2  | 12       | 0.36          |
| (2,1737) | 1:48:A:LEU:HD23  | 2:205:B:TRP:HZ2  | 12       | 0.36          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H    | 5        | 0.36          |
| (2,1415) | 1:70:A:ILE:HB    | 2:218:B:LEU:H    | 9        | 0.36          |
| (2,1407) | 2:213:B:PRO:HG2  | 2:214:B:LEU:H    | 18       | 0.36          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 18       | 0.36          |
| (2,1340) | 2:205:B:TRP:HE3  | 2:219:B:THR:H    | 16       | 0.36          |
| (2,1237) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB2  | 8        | 0.36          |
| (2,1145) | 2:205:B:TRP:HE3  | 2:219:B:THR:HA   | 9        | 0.36          |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG21 | 15       | 0.36          |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG22 | 15       | 0.36          |
| (2,1137) | 1:70:A:ILE:H     | 2:219:B:THR:HG23 | 15       | 0.36          |
| (2,720)  | 1:74:A:PHE:H     | 2:215:B:LYS:HG2  | 18       | 0.36          |
| (1,18)   | 1:53:A:HIS:O     | 1:57:A:SER:H     | 9        | 0.36          |
| (1,12)   | 1:50:A:ARG:O     | 1:54:A:ILE:H     | 20       | 0.36          |
| (1,9)    | 1:49:A:GLY:O     | 1:53:A:HIS:N     | 4        | 0.36          |
| (2,2222) | 2:218:B:LEU:HD11 | 2:219:B:THR:H    | 20       | 0.35          |
| (2,2222) | 2:218:B:LEU:HD12 | 2:219:B:THR:H    | 20       | 0.35          |
| (2,2222) | 2:218:B:LEU:HD13 | 2:219:B:THR:H    | 20       | 0.35          |
| (2,2222) | 2:218:B:LEU:HD21 | 2:219:B:THR:H    | 20       | 0.35          |
| (2,2222) | 2:218:B:LEU:HD22 | 2:219:B:THR:H    | 20       | 0.35          |
| (2,2222) | 2:218:B:LEU:HD23 | 2:219:B:THR:H    | 20       | 0.35          |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD11 | 9        | 0.35          |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD12 | 9        | 0.35          |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD13 | 9        | 0.35          |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD21 | 9        | 0.35          |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD22 | 9        | 0.35          |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD23 | 9        | 0.35          |
| (2,2109) | 2:206:B:ARG:HG2  | 2:220:B:ARG:HA   | 13       | 0.35          |
| (2,2109) | 2:206:B:ARG:HG3  | 2:220:B:ARG:HA   | 13       | 0.35          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD11 | 17       | 0.35          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD12 | 17       | 0.35          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD13 | 17       | 0.35          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD21 | 17       | 0.35          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD22 | 17       | 0.35          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD23 | 17       | 0.35          |
| (2,1909) | 1:69:A:GLU:HG2   | 2:219:B:THR:HB   | 11       | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1909) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 11       | 0.35          |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 18       | 0.35          |
| (2,1398) | 1:68:A:ASP:HB2   | 2:220:B:ARG:H    | 4        | 0.35          |
| (2,1386) | 2:204:B:THR:HB   | 2:205:B:TRP:H    | 18       | 0.35          |
| (2,1383) | 2:206:B:ARG:H    | 2:220:B:ARG:HA   | 14       | 0.35          |
| (2,1358) | 2:205:B:TRP:HD1  | 2:206:B:ARG:H    | 16       | 0.35          |
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 4        | 0.35          |
| (2,1242) | 1:70:A:ILE:H     | 2:219:B:THR:HA   | 5        | 0.35          |
| (2,1167) | 2:210:B:SER:H    | 2:215:B:LYS:HB2  | 12       | 0.35          |
| (2,763)  | 1:78:A:LYS:H     | 1:78:A:LYS:HD2   | 18       | 0.35          |
| (2,14)   | 1:70:A:ILE:HD11  | 2:205:B:TRP:HZ3  | 19       | 0.35          |
| (2,14)   | 1:70:A:ILE:HD12  | 2:205:B:TRP:HZ3  | 19       | 0.35          |
| (2,14)   | 1:70:A:ILE:HD13  | 2:205:B:TRP:HZ3  | 19       | 0.35          |
| (1,3)    | 1:34:A:ARG:O     | 1:38:A:LEU:N     | 15       | 0.35          |
| (2,2123) | 2:207:B:VAL:HG11 | 2:217:B:ARG:HA   | 19       | 0.34          |
| (2,2123) | 2:207:B:VAL:HG12 | 2:217:B:ARG:HA   | 19       | 0.34          |
| (2,2123) | 2:207:B:VAL:HG13 | 2:217:B:ARG:HA   | 19       | 0.34          |
| (2,2123) | 2:207:B:VAL:HG21 | 2:217:B:ARG:HA   | 19       | 0.34          |
| (2,2123) | 2:207:B:VAL:HG22 | 2:217:B:ARG:HA   | 19       | 0.34          |
| (2,2123) | 2:207:B:VAL:HG23 | 2:217:B:ARG:HA   | 19       | 0.34          |
| (2,2094) | 2:205:B:TRP:HE3  | 2:220:B:ARG:HB2  | 1        | 0.34          |
| (2,2094) | 2:205:B:TRP:HE3  | 2:220:B:ARG:HB3  | 1        | 0.34          |
| (2,1931) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG3  | 15       | 0.34          |
| (2,1931) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG3  | 15       | 0.34          |
| (2,1625) | 1:36:A:LEU:H     | 2:214:B:LEU:HD11 | 2        | 0.34          |
| (2,1625) | 1:36:A:LEU:H     | 2:214:B:LEU:HD12 | 2        | 0.34          |
| (2,1625) | 1:36:A:LEU:H     | 2:214:B:LEU:HD13 | 2        | 0.34          |
| (2,1625) | 1:36:A:LEU:H     | 2:214:B:LEU:HD21 | 2        | 0.34          |
| (2,1625) | 1:36:A:LEU:H     | 2:214:B:LEU:HD22 | 2        | 0.34          |
| (2,1625) | 1:36:A:LEU:H     | 2:214:B:LEU:HD23 | 2        | 0.34          |
| (2,1489) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE3  | 3        | 0.34          |
| (2,1438) | 2:203:B:LEU:HD11 | 2:204:B:THR:H    | 1        | 0.34          |
| (2,1438) | 2:203:B:LEU:HD12 | 2:204:B:THR:H    | 1        | 0.34          |
| (2,1438) | 2:203:B:LEU:HD13 | 2:204:B:THR:H    | 1        | 0.34          |
| (2,1428) | 2:208:B:GLN:H    | 2:219:B:THR:HG21 | 7        | 0.34          |
| (2,1428) | 2:208:B:GLN:H    | 2:219:B:THR:HG22 | 7        | 0.34          |
| (2,1428) | 2:208:B:GLN:H    | 2:219:B:THR:HG23 | 7        | 0.34          |
| (2,1427) | 2:215:B:LYS:H    | 2:215:B:LYS:HG3  | 20       | 0.34          |
| (2,1268) | 2:205:B:TRP:HA   | 2:220:B:ARG:HB3  | 10       | 0.34          |
| (2,1249) | 1:75:A:GLU:H     | 2:214:B:LEU:HD11 | 15       | 0.34          |
| (2,1249) | 1:75:A:GLU:H     | 2:214:B:LEU:HD12 | 15       | 0.34          |
| (2,1249) | 1:75:A:GLU:H     | 2:214:B:LEU:HD13 | 15       | 0.34          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1127) | 1:70:A:ILE:H    | 2:205:B:TRP:HH2  | 12       | 0.34          |
| (2,802)  | 1:74:A:PHE:H    | 2:214:B:LEU:HB3  | 9        | 0.34          |
| (2,720)  | 1:74:A:PHE:H    | 2:215:B:LYS:HG2  | 17       | 0.34          |
| (1,13)   | 1:51:A:VAL:O    | 1:55:A:ILE:N     | 9        | 0.34          |
| (1,13)   | 1:51:A:VAL:O    | 1:55:A:ILE:N     | 19       | 0.34          |
| (1,12)   | 1:50:A:ARG:O    | 1:54:A:ILE:H     | 7        | 0.34          |
| (2,2191) | 2:213:B:PRO:HB2 | 2:214:B:LEU:HD11 | 14       | 0.33          |
| (2,2191) | 2:213:B:PRO:HB2 | 2:214:B:LEU:HD12 | 14       | 0.33          |
| (2,2191) | 2:213:B:PRO:HB2 | 2:214:B:LEU:HD13 | 14       | 0.33          |
| (2,2191) | 2:213:B:PRO:HB2 | 2:214:B:LEU:HD21 | 14       | 0.33          |
| (2,2191) | 2:213:B:PRO:HB2 | 2:214:B:LEU:HD22 | 14       | 0.33          |
| (2,2191) | 2:213:B:PRO:HB2 | 2:214:B:LEU:HD23 | 14       | 0.33          |
| (2,2191) | 2:213:B:PRO:HB3 | 2:214:B:LEU:HD11 | 14       | 0.33          |
| (2,2191) | 2:213:B:PRO:HB3 | 2:214:B:LEU:HD12 | 14       | 0.33          |
| (2,2191) | 2:213:B:PRO:HB3 | 2:214:B:LEU:HD13 | 14       | 0.33          |
| (2,2191) | 2:213:B:PRO:HB3 | 2:214:B:LEU:HD21 | 14       | 0.33          |
| (2,2191) | 2:213:B:PRO:HB3 | 2:214:B:LEU:HD22 | 14       | 0.33          |
| (2,2191) | 2:213:B:PRO:HB3 | 2:214:B:LEU:HD23 | 14       | 0.33          |
| (2,2132) | 2:208:B:GLN:H   | 2:218:B:LEU:HD11 | 4        | 0.33          |
| (2,2132) | 2:208:B:GLN:H   | 2:218:B:LEU:HD12 | 4        | 0.33          |
| (2,2132) | 2:208:B:GLN:H   | 2:218:B:LEU:HD13 | 4        | 0.33          |
| (2,2132) | 2:208:B:GLN:H   | 2:218:B:LEU:HD21 | 4        | 0.33          |
| (2,2132) | 2:208:B:GLN:H   | 2:218:B:LEU:HD22 | 4        | 0.33          |
| (2,2132) | 2:208:B:GLN:H   | 2:218:B:LEU:HD23 | 4        | 0.33          |
| (2,2112) | 2:206:B:ARG:HD2 | 2:207:B:VAL:H    | 10       | 0.33          |
| (2,2112) | 2:206:B:ARG:HD3 | 2:207:B:VAL:H    | 10       | 0.33          |
| (2,1957) | 1:76:A:THR:H    | 2:214:B:LEU:HD11 | 13       | 0.33          |
| (2,1957) | 1:76:A:THR:H    | 2:214:B:LEU:HD12 | 13       | 0.33          |
| (2,1957) | 1:76:A:THR:H    | 2:214:B:LEU:HD13 | 13       | 0.33          |
| (2,1957) | 1:76:A:THR:H    | 2:214:B:LEU:HD21 | 13       | 0.33          |
| (2,1957) | 1:76:A:THR:H    | 2:214:B:LEU:HD22 | 13       | 0.33          |
| (2,1957) | 1:76:A:THR:H    | 2:214:B:LEU:HD23 | 13       | 0.33          |
| (2,1929) | 1:73:A:ASP:HB2  | 2:215:B:LYS:HA   | 9        | 0.33          |
| (2,1929) | 1:73:A:ASP:HB3  | 2:215:B:LYS:HA   | 9        | 0.33          |
| (2,1909) | 1:69:A:GLU:HG2  | 2:219:B:THR:HB   | 14       | 0.33          |
| (2,1909) | 1:69:A:GLU:HG3  | 2:219:B:THR:HB   | 14       | 0.33          |
| (2,1738) | 1:48:A:LEU:HD11 | 2:206:B:ARG:H    | 4        | 0.33          |
| (2,1738) | 1:48:A:LEU:HD12 | 2:206:B:ARG:H    | 4        | 0.33          |
| (2,1738) | 1:48:A:LEU:HD13 | 2:206:B:ARG:H    | 4        | 0.33          |
| (2,1738) | 1:48:A:LEU:HD21 | 2:206:B:ARG:H    | 4        | 0.33          |
| (2,1738) | 1:48:A:LEU:HD22 | 2:206:B:ARG:H    | 4        | 0.33          |
| (2,1738) | 1:48:A:LEU:HD23 | 2:206:B:ARG:H    | 4        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 3        | 0.33          |
| (2,1233) | 2:204:B:THR:HG21 | 2:205:B:TRP:HB3  | 14       | 0.33          |
| (2,1233) | 2:204:B:THR:HG22 | 2:205:B:TRP:HB3  | 14       | 0.33          |
| (2,1233) | 2:204:B:THR:HG23 | 2:205:B:TRP:HB3  | 14       | 0.33          |
| (2,1215) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD21 | 19       | 0.33          |
| (2,1215) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD22 | 19       | 0.33          |
| (2,1215) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD23 | 19       | 0.33          |
| (2,1131) | 1:72:A:ILE:H     | 2:217:B:ARG:HB2  | 11       | 0.33          |
| (2,1127) | 1:70:A:ILE:H     | 2:205:B:TRP:HH2  | 11       | 0.33          |
| (2,1104) | 1:73:A:ASP:H     | 2:215:B:LYS:HA   | 14       | 0.33          |
| (2,801)  | 1:74:A:PHE:H     | 2:214:B:LEU:HB2  | 15       | 0.33          |
| (2,799)  | 1:22:A:GLU:HB2   | 1:23:A:GLU:H     | 19       | 0.33          |
| (2,738)  | 1:33:A:LYS:H     | 1:33:A:LYS:HD2   | 8        | 0.33          |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD11 | 16       | 0.33          |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD12 | 16       | 0.33          |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD13 | 16       | 0.33          |
| (2,189)  | 1:70:A:ILE:HG12  | 2:205:B:TRP:HH2  | 7        | 0.33          |
| (2,101)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HH2  | 17       | 0.33          |
| (2,101)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HH2  | 17       | 0.33          |
| (2,101)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HH2  | 17       | 0.33          |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H     | 14       | 0.33          |
| (2,2172) | 2:210:B:SER:HB2  | 2:215:B:LYS:HD2  | 20       | 0.32          |
| (2,2172) | 2:210:B:SER:HB3  | 2:215:B:LYS:HD2  | 20       | 0.32          |
| (2,2105) | 2:206:B:ARG:HB2  | 2:207:B:VAL:H    | 11       | 0.32          |
| (2,2105) | 2:206:B:ARG:HB3  | 2:207:B:VAL:H    | 11       | 0.32          |
| (2,2100) | 2:206:B:ARG:H    | 2:206:B:ARG:HD2  | 2        | 0.32          |
| (2,2100) | 2:206:B:ARG:H    | 2:206:B:ARG:HD3  | 2        | 0.32          |
| (2,1950) | 1:75:A:GLU:H     | 2:214:B:LEU:HD11 | 13       | 0.32          |
| (2,1950) | 1:75:A:GLU:H     | 2:214:B:LEU:HD12 | 13       | 0.32          |
| (2,1950) | 1:75:A:GLU:H     | 2:214:B:LEU:HD13 | 13       | 0.32          |
| (2,1950) | 1:75:A:GLU:H     | 2:214:B:LEU:HD21 | 13       | 0.32          |
| (2,1950) | 1:75:A:GLU:H     | 2:214:B:LEU:HD22 | 13       | 0.32          |
| (2,1950) | 1:75:A:GLU:H     | 2:214:B:LEU:HD23 | 13       | 0.32          |
| (2,1438) | 2:203:B:LEU:HD11 | 2:204:B:THR:H    | 11       | 0.32          |
| (2,1438) | 2:203:B:LEU:HD12 | 2:204:B:THR:H    | 11       | 0.32          |
| (2,1438) | 2:203:B:LEU:HD13 | 2:204:B:THR:H    | 11       | 0.32          |
| (2,1392) | 2:209:B:ARG:HD3  | 2:210:B:SER:H    | 12       | 0.32          |
| (2,1391) | 2:209:B:ARG:HD2  | 2:210:B:SER:H    | 1        | 0.32          |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H    | 16       | 0.32          |
| (2,1347) | 2:208:B:GLN:H    | 2:217:B:ARG:H    | 18       | 0.32          |
| (2,1187) | 2:217:B:ARG:HG2  | 2:218:B:LEU:H    | 7        | 0.32          |
| (2,1114) | 1:37:A:SER:H     | 2:214:B:LEU:HA   | 20       | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,147)  | 1:30:A:TYR:HA    | 2:214:B:LEU:HD21 | 18       | 0.32          |
| (2,147)  | 1:30:A:TYR:HA    | 2:214:B:LEU:HD22 | 18       | 0.32          |
| (2,147)  | 1:30:A:TYR:HA    | 2:214:B:LEU:HD23 | 18       | 0.32          |
| (2,2222) | 2:218:B:LEU:HD11 | 2:219:B:THR:H    | 2        | 0.31          |
| (2,2222) | 2:218:B:LEU:HD12 | 2:219:B:THR:H    | 2        | 0.31          |
| (2,2222) | 2:218:B:LEU:HD13 | 2:219:B:THR:H    | 2        | 0.31          |
| (2,2222) | 2:218:B:LEU:HD21 | 2:219:B:THR:H    | 2        | 0.31          |
| (2,2222) | 2:218:B:LEU:HD22 | 2:219:B:THR:H    | 2        | 0.31          |
| (2,2222) | 2:218:B:LEU:HD23 | 2:219:B:THR:H    | 2        | 0.31          |
| (2,2222) | 2:218:B:LEU:HD11 | 2:219:B:THR:H    | 6        | 0.31          |
| (2,2222) | 2:218:B:LEU:HD12 | 2:219:B:THR:H    | 6        | 0.31          |
| (2,2222) | 2:218:B:LEU:HD13 | 2:219:B:THR:H    | 6        | 0.31          |
| (2,2222) | 2:218:B:LEU:HD21 | 2:219:B:THR:H    | 6        | 0.31          |
| (2,2222) | 2:218:B:LEU:HD22 | 2:219:B:THR:H    | 6        | 0.31          |
| (2,2222) | 2:218:B:LEU:HD23 | 2:219:B:THR:H    | 6        | 0.31          |
| (2,2222) | 2:218:B:LEU:HD11 | 2:219:B:THR:H    | 17       | 0.31          |
| (2,2222) | 2:218:B:LEU:HD12 | 2:219:B:THR:H    | 17       | 0.31          |
| (2,2222) | 2:218:B:LEU:HD13 | 2:219:B:THR:H    | 17       | 0.31          |
| (2,2222) | 2:218:B:LEU:HD21 | 2:219:B:THR:H    | 17       | 0.31          |
| (2,2222) | 2:218:B:LEU:HD22 | 2:219:B:THR:H    | 17       | 0.31          |
| (2,2222) | 2:218:B:LEU:HD23 | 2:219:B:THR:H    | 17       | 0.31          |
| (2,2216) | 2:217:B:ARG:HD2  | 2:219:B:THR:HB   | 10       | 0.31          |
| (2,2216) | 2:217:B:ARG:HD3  | 2:219:B:THR:HB   | 10       | 0.31          |
| (2,2184) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HB3  | 7        | 0.31          |
| (2,2184) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB3  | 7        | 0.31          |
| (2,2127) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HG   | 19       | 0.31          |
| (2,2127) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HG   | 19       | 0.31          |
| (2,2127) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HG   | 19       | 0.31          |
| (2,2127) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HG   | 19       | 0.31          |
| (2,2127) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HG   | 19       | 0.31          |
| (2,2127) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HG   | 19       | 0.31          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD11 | 17       | 0.31          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD12 | 17       | 0.31          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD13 | 17       | 0.31          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD21 | 17       | 0.31          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD22 | 17       | 0.31          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD23 | 17       | 0.31          |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD11 | 14       | 0.31          |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD12 | 14       | 0.31          |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD13 | 14       | 0.31          |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD21 | 14       | 0.31          |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD22 | 14       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD23 | 14       | 0.31          |
| (2,1416) | 2:215:B:LYS:H    | 2:215:B:LYS:HB2  | 10       | 0.31          |
| (2,1415) | 1:70:A:ILE:HB    | 2:218:B:LEU:H    | 5        | 0.31          |
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 6        | 0.31          |
| (2,1174) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HB2  | 3        | 0.31          |
| (2,597)  | 1:86:A:GLU:HA    | 1:89:A:VAL:HB    | 15       | 0.31          |
| (2,22)   | 1:43:A:LEU:HD21  | 1:88:A:TYR:HD1   | 10       | 0.31          |
| (2,22)   | 1:43:A:LEU:HD21  | 1:88:A:TYR:HD2   | 10       | 0.31          |
| (2,22)   | 1:43:A:LEU:HD22  | 1:88:A:TYR:HD1   | 10       | 0.31          |
| (2,22)   | 1:43:A:LEU:HD22  | 1:88:A:TYR:HD2   | 10       | 0.31          |
| (2,22)   | 1:43:A:LEU:HD23  | 1:88:A:TYR:HD1   | 10       | 0.31          |
| (2,22)   | 1:43:A:LEU:HD23  | 1:88:A:TYR:HD2   | 10       | 0.31          |
| (1,18)   | 1:53:A:HIS:O     | 1:57:A:SER:H     | 10       | 0.31          |
| (2,2222) | 2:218:B:LEU:HD11 | 2:219:B:THR:H    | 12       | 0.3           |
| (2,2222) | 2:218:B:LEU:HD12 | 2:219:B:THR:H    | 12       | 0.3           |
| (2,2222) | 2:218:B:LEU:HD13 | 2:219:B:THR:H    | 12       | 0.3           |
| (2,2222) | 2:218:B:LEU:HD21 | 2:219:B:THR:H    | 12       | 0.3           |
| (2,2222) | 2:218:B:LEU:HD22 | 2:219:B:THR:H    | 12       | 0.3           |
| (2,2222) | 2:218:B:LEU:HD23 | 2:219:B:THR:H    | 12       | 0.3           |
| (2,2222) | 2:218:B:LEU:HD11 | 2:219:B:THR:H    | 14       | 0.3           |
| (2,2222) | 2:218:B:LEU:HD12 | 2:219:B:THR:H    | 14       | 0.3           |
| (2,2222) | 2:218:B:LEU:HD13 | 2:219:B:THR:H    | 14       | 0.3           |
| (2,2222) | 2:218:B:LEU:HD21 | 2:219:B:THR:H    | 14       | 0.3           |
| (2,2222) | 2:218:B:LEU:HD22 | 2:219:B:THR:H    | 14       | 0.3           |
| (2,2222) | 2:218:B:LEU:HD23 | 2:219:B:THR:H    | 14       | 0.3           |
| (2,2165) | 2:209:B:ARG:HD2  | 2:210:B:SER:H    | 12       | 0.3           |
| (2,2165) | 2:209:B:ARG:HD3  | 2:210:B:SER:H    | 12       | 0.3           |
| (2,2141) | 2:208:B:GLN:HB2  | 2:219:B:THR:H    | 13       | 0.3           |
| (2,2141) | 2:208:B:GLN:HB3  | 2:219:B:THR:H    | 13       | 0.3           |
| (2,2103) | 2:206:B:ARG:H    | 2:221:B:GLU:HG2  | 9        | 0.3           |
| (2,2103) | 2:206:B:ARG:H    | 2:221:B:GLU:HG3  | 9        | 0.3           |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD11 | 4        | 0.3           |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD12 | 4        | 0.3           |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD13 | 4        | 0.3           |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD21 | 4        | 0.3           |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD22 | 4        | 0.3           |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD23 | 4        | 0.3           |
| (2,1900) | 1:68:A:ASP:HA    | 2:220:B:ARG:HB2  | 1        | 0.3           |
| (2,1900) | 1:68:A:ASP:HA    | 2:220:B:ARG:HB3  | 1        | 0.3           |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD11 | 5        | 0.3           |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD12 | 5        | 0.3           |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD13 | 5        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD21 | 5        | 0.3           |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD22 | 5        | 0.3           |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD23 | 5        | 0.3           |
| (2,1545) | 1:28:A:MET:HE1   | 1:33:A:LYS:HG2   | 9        | 0.3           |
| (2,1545) | 1:28:A:MET:HE1   | 1:33:A:LYS:HG3   | 9        | 0.3           |
| (2,1545) | 1:28:A:MET:HE2   | 1:33:A:LYS:HG2   | 9        | 0.3           |
| (2,1545) | 1:28:A:MET:HE2   | 1:33:A:LYS:HG3   | 9        | 0.3           |
| (2,1545) | 1:28:A:MET:HE3   | 1:33:A:LYS:HG2   | 9        | 0.3           |
| (2,1545) | 1:28:A:MET:HE3   | 1:33:A:LYS:HG3   | 9        | 0.3           |
| (2,1475) | 1:73:A:ASP:HA    | 2:216:B:ILE:H    | 2        | 0.3           |
| (2,1435) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H    | 5        | 0.3           |
| (2,1435) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H    | 5        | 0.3           |
| (2,1435) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H    | 5        | 0.3           |
| (2,1415) | 1:70:A:ILE:HB    | 2:218:B:LEU:H    | 11       | 0.3           |
| (2,1403) | 2:221:B:GLU:HB3  | 2:222:B:ALA:H    | 5        | 0.3           |
| (2,1386) | 2:204:B:THR:HB   | 2:205:B:TRP:H    | 2        | 0.3           |
| (2,1358) | 2:205:B:TRP:HD1  | 2:206:B:ARG:H    | 7        | 0.3           |
| (2,1357) | 2:205:B:TRP:H    | 2:205:B:TRP:HD1  | 3        | 0.3           |
| (2,1261) | 2:214:B:LEU:HA   | 2:215:B:LYS:HB2  | 10       | 0.3           |
| (2,1237) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB2  | 16       | 0.3           |
| (2,1225) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HA   | 19       | 0.3           |
| (2,32)   | 1:30:A:TYR:HE1   | 2:214:B:LEU:HD21 | 9        | 0.3           |
| (2,32)   | 1:30:A:TYR:HE1   | 2:214:B:LEU:HD22 | 9        | 0.3           |
| (2,32)   | 1:30:A:TYR:HE1   | 2:214:B:LEU:HD23 | 9        | 0.3           |
| (2,32)   | 1:30:A:TYR:HE2   | 2:214:B:LEU:HD21 | 9        | 0.3           |
| (2,32)   | 1:30:A:TYR:HE2   | 2:214:B:LEU:HD22 | 9        | 0.3           |
| (2,32)   | 1:30:A:TYR:HE2   | 2:214:B:LEU:HD23 | 9        | 0.3           |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 4        | 0.3           |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 11       | 0.3           |
| (2,2189) | 2:213:B:PRO:HA   | 2:214:B:LEU:HD11 | 14       | 0.29          |
| (2,2189) | 2:213:B:PRO:HA   | 2:214:B:LEU:HD12 | 14       | 0.29          |
| (2,2189) | 2:213:B:PRO:HA   | 2:214:B:LEU:HD13 | 14       | 0.29          |
| (2,2189) | 2:213:B:PRO:HA   | 2:214:B:LEU:HD21 | 14       | 0.29          |
| (2,2189) | 2:213:B:PRO:HA   | 2:214:B:LEU:HD22 | 14       | 0.29          |
| (2,2189) | 2:213:B:PRO:HA   | 2:214:B:LEU:HD23 | 14       | 0.29          |
| (2,2184) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HB3  | 16       | 0.29          |
| (2,2184) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB3  | 16       | 0.29          |
| (2,1930) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG2  | 11       | 0.29          |
| (2,1930) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG2  | 11       | 0.29          |
| (2,1737) | 1:48:A:LEU:HD11  | 2:205:B:TRP:HZ2  | 17       | 0.29          |
| (2,1737) | 1:48:A:LEU:HD12  | 2:205:B:TRP:HZ2  | 17       | 0.29          |
| (2,1737) | 1:48:A:LEU:HD13  | 2:205:B:TRP:HZ2  | 17       | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1737) | 1:48:A:LEU:HD21  | 2:205:B:TRP:HZ2  | 17       | 0.29          |
| (2,1737) | 1:48:A:LEU:HD22  | 2:205:B:TRP:HZ2  | 17       | 0.29          |
| (2,1737) | 1:48:A:LEU:HD23  | 2:205:B:TRP:HZ2  | 17       | 0.29          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD11 | 2        | 0.29          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD12 | 2        | 0.29          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD13 | 2        | 0.29          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD21 | 2        | 0.29          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD22 | 2        | 0.29          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD23 | 2        | 0.29          |
| (2,1546) | 1:28:A:MET:HE1   | 1:33:A:LYS:HD2   | 11       | 0.29          |
| (2,1546) | 1:28:A:MET:HE1   | 1:33:A:LYS:HD3   | 11       | 0.29          |
| (2,1546) | 1:28:A:MET:HE2   | 1:33:A:LYS:HD2   | 11       | 0.29          |
| (2,1546) | 1:28:A:MET:HE2   | 1:33:A:LYS:HD3   | 11       | 0.29          |
| (2,1546) | 1:28:A:MET:HE3   | 1:33:A:LYS:HD2   | 11       | 0.29          |
| (2,1546) | 1:28:A:MET:HE3   | 1:33:A:LYS:HD3   | 11       | 0.29          |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG   | 14       | 0.29          |
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 10       | 0.29          |
| (2,1174) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HB2  | 6        | 0.29          |
| (2,1102) | 1:75:A:GLU:H     | 2:215:B:LYS:HA   | 20       | 0.29          |
| (2,407)  | 1:52:A:VAL:HB    | 1:70:A:ILE:HG21  | 17       | 0.29          |
| (2,407)  | 1:52:A:VAL:HB    | 1:70:A:ILE:HG22  | 17       | 0.29          |
| (2,407)  | 1:52:A:VAL:HB    | 1:70:A:ILE:HG23  | 17       | 0.29          |
| (2,189)  | 1:70:A:ILE:HG12  | 2:205:B:TRP:HH2  | 12       | 0.29          |
| (2,147)  | 1:30:A:TYR:HA    | 2:214:B:LEU:HD21 | 17       | 0.29          |
| (2,147)  | 1:30:A:TYR:HA    | 2:214:B:LEU:HD22 | 17       | 0.29          |
| (2,147)  | 1:30:A:TYR:HA    | 2:214:B:LEU:HD23 | 17       | 0.29          |
| (1,18)   | 1:53:A:HIS:O     | 1:57:A:SER:H     | 17       | 0.29          |
| (1,17)   | 1:53:A:HIS:O     | 1:57:A:SER:N     | 8        | 0.29          |
| (2,2222) | 2:218:B:LEU:HD11 | 2:219:B:THR:H    | 7        | 0.28          |
| (2,2222) | 2:218:B:LEU:HD12 | 2:219:B:THR:H    | 7        | 0.28          |
| (2,2222) | 2:218:B:LEU:HD13 | 2:219:B:THR:H    | 7        | 0.28          |
| (2,2222) | 2:218:B:LEU:HD21 | 2:219:B:THR:H    | 7        | 0.28          |
| (2,2222) | 2:218:B:LEU:HD22 | 2:219:B:THR:H    | 7        | 0.28          |
| (2,2222) | 2:218:B:LEU:HD23 | 2:219:B:THR:H    | 7        | 0.28          |
| (2,2184) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HB3  | 6        | 0.28          |
| (2,2184) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB3  | 6        | 0.28          |
| (2,2142) | 2:208:B:GLN:HB2  | 2:219:B:THR:HG21 | 19       | 0.28          |
| (2,2142) | 2:208:B:GLN:HB2  | 2:219:B:THR:HG22 | 19       | 0.28          |
| (2,2142) | 2:208:B:GLN:HB2  | 2:219:B:THR:HG23 | 19       | 0.28          |
| (2,2142) | 2:208:B:GLN:HB3  | 2:219:B:THR:HG21 | 19       | 0.28          |
| (2,2142) | 2:208:B:GLN:HB3  | 2:219:B:THR:HG22 | 19       | 0.28          |
| (2,2142) | 2:208:B:GLN:HB3  | 2:219:B:THR:HG23 | 19       | 0.28          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2140) | 2:208:B:GLN:HB2 | 2:217:B:ARG:HD2  | 11       | 0.28          |
| (2,2140) | 2:208:B:GLN:HB2 | 2:217:B:ARG:HD3  | 11       | 0.28          |
| (2,2140) | 2:208:B:GLN:HB3 | 2:217:B:ARG:HD2  | 11       | 0.28          |
| (2,2140) | 2:208:B:GLN:HB3 | 2:217:B:ARG:HD3  | 11       | 0.28          |
| (2,2113) | 2:206:B:ARG:HD2 | 2:221:B:GLU:HG2  | 14       | 0.28          |
| (2,2113) | 2:206:B:ARG:HD2 | 2:221:B:GLU:HG3  | 14       | 0.28          |
| (2,2113) | 2:206:B:ARG:HD3 | 2:221:B:GLU:HG2  | 14       | 0.28          |
| (2,2113) | 2:206:B:ARG:HD3 | 2:221:B:GLU:HG3  | 14       | 0.28          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD11 | 11       | 0.28          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD12 | 11       | 0.28          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD13 | 11       | 0.28          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD21 | 11       | 0.28          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD22 | 11       | 0.28          |
| (2,2101) | 2:206:B:ARG:H   | 2:218:B:LEU:HD23 | 11       | 0.28          |
| (2,2093) | 2:205:B:TRP:HE3 | 2:218:B:LEU:HD11 | 20       | 0.28          |
| (2,2093) | 2:205:B:TRP:HE3 | 2:218:B:LEU:HD12 | 20       | 0.28          |
| (2,2093) | 2:205:B:TRP:HE3 | 2:218:B:LEU:HD13 | 20       | 0.28          |
| (2,2093) | 2:205:B:TRP:HE3 | 2:218:B:LEU:HD21 | 20       | 0.28          |
| (2,2093) | 2:205:B:TRP:HE3 | 2:218:B:LEU:HD22 | 20       | 0.28          |
| (2,2093) | 2:205:B:TRP:HE3 | 2:218:B:LEU:HD23 | 20       | 0.28          |
| (2,1954) | 1:75:A:GLU:HG2  | 2:214:B:LEU:HD11 | 7        | 0.28          |
| (2,1954) | 1:75:A:GLU:HG2  | 2:214:B:LEU:HD12 | 7        | 0.28          |
| (2,1954) | 1:75:A:GLU:HG2  | 2:214:B:LEU:HD13 | 7        | 0.28          |
| (2,1954) | 1:75:A:GLU:HG2  | 2:214:B:LEU:HD21 | 7        | 0.28          |
| (2,1954) | 1:75:A:GLU:HG2  | 2:214:B:LEU:HD22 | 7        | 0.28          |
| (2,1954) | 1:75:A:GLU:HG2  | 2:214:B:LEU:HD23 | 7        | 0.28          |
| (2,1799) | 1:52:A:VAL:HG11 | 2:218:B:LEU:HD11 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG11 | 2:218:B:LEU:HD12 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG11 | 2:218:B:LEU:HD13 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG11 | 2:218:B:LEU:HD21 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG11 | 2:218:B:LEU:HD22 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG11 | 2:218:B:LEU:HD23 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG12 | 2:218:B:LEU:HD11 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG12 | 2:218:B:LEU:HD12 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG12 | 2:218:B:LEU:HD13 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG12 | 2:218:B:LEU:HD21 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG12 | 2:218:B:LEU:HD22 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG12 | 2:218:B:LEU:HD23 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG13 | 2:218:B:LEU:HD11 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG13 | 2:218:B:LEU:HD12 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG13 | 2:218:B:LEU:HD13 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG13 | 2:218:B:LEU:HD21 | 18       | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1799) | 1:52:A:VAL:HG13  | 2:218:B:LEU:HD22 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG13  | 2:218:B:LEU:HD23 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG21  | 2:218:B:LEU:HD11 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG21  | 2:218:B:LEU:HD12 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG21  | 2:218:B:LEU:HD13 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG21  | 2:218:B:LEU:HD21 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG21  | 2:218:B:LEU:HD22 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG21  | 2:218:B:LEU:HD23 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG22  | 2:218:B:LEU:HD11 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG22  | 2:218:B:LEU:HD12 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG22  | 2:218:B:LEU:HD13 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG22  | 2:218:B:LEU:HD21 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG22  | 2:218:B:LEU:HD22 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG22  | 2:218:B:LEU:HD23 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG23  | 2:218:B:LEU:HD11 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG23  | 2:218:B:LEU:HD12 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG23  | 2:218:B:LEU:HD13 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG23  | 2:218:B:LEU:HD21 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG23  | 2:218:B:LEU:HD22 | 18       | 0.28          |
| (2,1799) | 1:52:A:VAL:HG23  | 2:218:B:LEU:HD23 | 18       | 0.28          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD11 | 14       | 0.28          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD12 | 14       | 0.28          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD13 | 14       | 0.28          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD21 | 14       | 0.28          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD22 | 14       | 0.28          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD23 | 14       | 0.28          |
| (2,1546) | 1:28:A:MET:HE1   | 1:33:A:LYS:HD2   | 10       | 0.28          |
| (2,1546) | 1:28:A:MET:HE1   | 1:33:A:LYS:HD3   | 10       | 0.28          |
| (2,1546) | 1:28:A:MET:HE2   | 1:33:A:LYS:HD2   | 10       | 0.28          |
| (2,1546) | 1:28:A:MET:HE2   | 1:33:A:LYS:HD3   | 10       | 0.28          |
| (2,1546) | 1:28:A:MET:HE3   | 1:33:A:LYS:HD2   | 10       | 0.28          |
| (2,1546) | 1:28:A:MET:HE3   | 1:33:A:LYS:HD3   | 10       | 0.28          |
| (2,1475) | 1:73:A:ASP:HA    | 2:216:B:ILE:H    | 14       | 0.28          |
| (2,1398) | 1:68:A:ASP:HB2   | 2:220:B:ARG:H    | 3        | 0.28          |
| (2,1359) | 2:205:B:TRP:HE3  | 2:206:B:ARG:H    | 12       | 0.28          |
| (2,1331) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD21 | 9        | 0.28          |
| (2,1331) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD22 | 9        | 0.28          |
| (2,1331) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD23 | 9        | 0.28          |
| (2,1294) | 2:204:B:THR:HG21 | 2:205:B:TRP:HD1  | 16       | 0.28          |
| (2,1294) | 2:204:B:THR:HG22 | 2:205:B:TRP:HD1  | 16       | 0.28          |
| (2,1294) | 2:204:B:THR:HG23 | 2:205:B:TRP:HD1  | 16       | 0.28          |
| (2,1256) | 1:73:A:ASP:HA    | 2:215:B:LYS:HB3  | 20       | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1237) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB2  | 11       | 0.28          |
| (2,1202) | 2:215:B:LYS:HG2  | 2:216:B:ILE:H    | 18       | 0.28          |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD11 | 3        | 0.28          |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD12 | 3        | 0.28          |
| (2,1193) | 2:207:B:VAL:HA   | 2:218:B:LEU:HD13 | 3        | 0.28          |
| (2,1152) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HA   | 3        | 0.28          |
| (2,1152) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HA   | 3        | 0.28          |
| (2,679)  | 1:34:A:ARG:H     | 2:214:B:LEU:HD11 | 6        | 0.28          |
| (2,679)  | 1:34:A:ARG:H     | 2:214:B:LEU:HD12 | 6        | 0.28          |
| (2,679)  | 1:34:A:ARG:H     | 2:214:B:LEU:HD13 | 6        | 0.28          |
| (1,12)   | 1:50:A:ARG:O     | 1:54:A:ILE:H     | 17       | 0.28          |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H     | 7        | 0.28          |
| (1,9)    | 1:49:A:GLY:O     | 1:53:A:HIS:N     | 14       | 0.28          |
| (1,9)    | 1:49:A:GLY:O     | 1:53:A:HIS:N     | 16       | 0.28          |
| (2,2222) | 2:218:B:LEU:HD11 | 2:219:B:THR:H    | 9        | 0.27          |
| (2,2222) | 2:218:B:LEU:HD12 | 2:219:B:THR:H    | 9        | 0.27          |
| (2,2222) | 2:218:B:LEU:HD13 | 2:219:B:THR:H    | 9        | 0.27          |
| (2,2222) | 2:218:B:LEU:HD21 | 2:219:B:THR:H    | 9        | 0.27          |
| (2,2222) | 2:218:B:LEU:HD22 | 2:219:B:THR:H    | 9        | 0.27          |
| (2,2222) | 2:218:B:LEU:HD23 | 2:219:B:THR:H    | 9        | 0.27          |
| (2,2128) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HD11 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HD12 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HD13 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HD21 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HD22 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HD23 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HD11 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HD12 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HD13 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HD21 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HD22 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HD23 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HD11 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HD12 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HD13 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HD21 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HD22 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HD23 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HD11 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HD12 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HD13 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HD21 | 18       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2128) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HD22 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HD23 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HD11 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HD12 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HD13 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HD21 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HD22 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HD23 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HD11 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HD12 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HD13 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HD21 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HD22 | 18       | 0.27          |
| (2,2128) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HD23 | 18       | 0.27          |
| (2,2122) | 2:207:B:VAL:HG11 | 2:217:B:ARG:H    | 8        | 0.27          |
| (2,2122) | 2:207:B:VAL:HG12 | 2:217:B:ARG:H    | 8        | 0.27          |
| (2,2122) | 2:207:B:VAL:HG13 | 2:217:B:ARG:H    | 8        | 0.27          |
| (2,2122) | 2:207:B:VAL:HG21 | 2:217:B:ARG:H    | 8        | 0.27          |
| (2,2122) | 2:207:B:VAL:HG22 | 2:217:B:ARG:H    | 8        | 0.27          |
| (2,2122) | 2:207:B:VAL:HG23 | 2:217:B:ARG:H    | 8        | 0.27          |
| (2,2109) | 2:206:B:ARG:HG2  | 2:220:B:ARG:HA   | 1        | 0.27          |
| (2,2109) | 2:206:B:ARG:HG3  | 2:220:B:ARG:HA   | 1        | 0.27          |
| (2,2050) | 1:90:A:LYS:HA    | 1:90:A:LYS:HD2   | 16       | 0.27          |
| (2,2050) | 1:90:A:LYS:HA    | 1:90:A:LYS:HD3   | 16       | 0.27          |
| (2,2050) | 1:90:A:LYS:HA    | 1:90:A:LYS:HD2   | 17       | 0.27          |
| (2,2050) | 1:90:A:LYS:HA    | 1:90:A:LYS:HD3   | 17       | 0.27          |
| (2,1730) | 1:48:A:LEU:HB2   | 2:205:B:TRP:HH2  | 18       | 0.27          |
| (2,1730) | 1:48:A:LEU:HB3   | 2:205:B:TRP:HH2  | 18       | 0.27          |
| (2,1486) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB3  | 16       | 0.27          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H    | 17       | 0.27          |
| (2,1473) | 2:205:B:TRP:HB2  | 2:219:B:THR:H    | 16       | 0.27          |
| (2,1355) | 1:74:A:PHE:HD1   | 2:214:B:LEU:H    | 13       | 0.27          |
| (2,1355) | 1:74:A:PHE:HD2   | 2:214:B:LEU:H    | 13       | 0.27          |
| (2,1353) | 1:74:A:PHE:HD1   | 2:215:B:LYS:H    | 7        | 0.27          |
| (2,1353) | 1:74:A:PHE:HD2   | 2:215:B:LYS:H    | 7        | 0.27          |
| (2,1286) | 1:74:A:PHE:H     | 2:215:B:LYS:HG3  | 18       | 0.27          |
| (2,1250) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HG   | 13       | 0.27          |
| (2,1250) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HG   | 13       | 0.27          |
| (2,633)  | 1:71:A:GLU:HG3   | 2:217:B:ARG:HG2  | 12       | 0.27          |
| (2,617)  | 1:73:A:ASP:HA    | 2:215:B:LYS:HA   | 13       | 0.27          |
| (2,531)  | 1:76:A:THR:HG21  | 2:215:B:LYS:HD3  | 13       | 0.27          |
| (2,531)  | 1:76:A:THR:HG22  | 2:215:B:LYS:HD3  | 13       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,531)  | 1:76:A:THR:HG23  | 2:215:B:LYS:HD3  | 13       | 0.27          |
| (2,11)   | 2:204:B:THR:HA   | 2:205:B:TRP:HD1  | 20       | 0.27          |
| (1,17)   | 1:53:A:HIS:O     | 1:57:A:SER:N     | 9        | 0.27          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 19       | 0.27          |
| (1,13)   | 1:51:A:VAL:O     | 1:55:A:ILE:N     | 12       | 0.27          |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 13       | 0.27          |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H     | 2        | 0.27          |
| (1,4)    | 1:34:A:ARG:O     | 1:38:A:LEU:H     | 15       | 0.27          |
| (1,1)    | 1:33:A:LYS:O     | 1:37:A:SER:N     | 15       | 0.27          |
| (2,2212) | 2:217:B:ARG:HA   | 2:218:B:LEU:HD11 | 18       | 0.26          |
| (2,2212) | 2:217:B:ARG:HA   | 2:218:B:LEU:HD12 | 18       | 0.26          |
| (2,2212) | 2:217:B:ARG:HA   | 2:218:B:LEU:HD13 | 18       | 0.26          |
| (2,2212) | 2:217:B:ARG:HA   | 2:218:B:LEU:HD21 | 18       | 0.26          |
| (2,2212) | 2:217:B:ARG:HA   | 2:218:B:LEU:HD22 | 18       | 0.26          |
| (2,2212) | 2:217:B:ARG:HA   | 2:218:B:LEU:HD23 | 18       | 0.26          |
| (2,2199) | 2:214:B:LEU:HD11 | 2:215:B:LYS:H    | 5        | 0.26          |
| (2,2199) | 2:214:B:LEU:HD12 | 2:215:B:LYS:H    | 5        | 0.26          |
| (2,2199) | 2:214:B:LEU:HD13 | 2:215:B:LYS:H    | 5        | 0.26          |
| (2,2199) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H    | 5        | 0.26          |
| (2,2199) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H    | 5        | 0.26          |
| (2,2199) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H    | 5        | 0.26          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD11 | 13       | 0.26          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD12 | 13       | 0.26          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD13 | 13       | 0.26          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD21 | 13       | 0.26          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD22 | 13       | 0.26          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD23 | 13       | 0.26          |
| (2,2165) | 2:209:B:ARG:HD2  | 2:210:B:SER:H    | 3        | 0.26          |
| (2,2165) | 2:209:B:ARG:HD3  | 2:210:B:SER:H    | 3        | 0.26          |
| (2,2152) | 2:208:B:GLN:HG2  | 2:219:B:THR:H    | 20       | 0.26          |
| (2,2152) | 2:208:B:GLN:HG3  | 2:219:B:THR:H    | 20       | 0.26          |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD11 | 4        | 0.26          |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD12 | 4        | 0.26          |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD13 | 4        | 0.26          |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD21 | 4        | 0.26          |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD22 | 4        | 0.26          |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD23 | 4        | 0.26          |
| (2,1500) | 1:20:A:GLU:HB2   | 1:21:A:GLU:H     | 4        | 0.26          |
| (2,1500) | 1:20:A:GLU:HB3   | 1:21:A:GLU:H     | 4        | 0.26          |
| (2,1474) | 1:75:A:GLU:HG2   | 2:215:B:LYS:H    | 7        | 0.26          |
| (2,1457) | 2:205:B:TRP:HB2  | 2:221:B:GLU:H    | 12       | 0.26          |
| (2,1204) | 1:73:A:ASP:HA    | 2:215:B:LYS:HG2  | 12       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1104) | 1:73:A:ASP:H     | 2:215:B:LYS:HA   | 15       | 0.26          |
| (2,1042) | 1:21:A:GLU:H     | 1:22:A:GLU:H     | 10       | 0.26          |
| (2,177)  | 1:73:A:ASP:HA    | 2:216:B:ILE:HG21 | 19       | 0.26          |
| (2,177)  | 1:73:A:ASP:HA    | 2:216:B:ILE:HG22 | 19       | 0.26          |
| (2,177)  | 1:73:A:ASP:HA    | 2:216:B:ILE:HG23 | 19       | 0.26          |
| (2,152)  | 1:34:A:ARG:HA    | 2:214:B:LEU:HG   | 20       | 0.26          |
| (1,21)   | 1:87:A:ARG:O     | 1:91:A:SER:N     | 13       | 0.26          |
| (1,17)   | 1:53:A:HIS:O     | 1:57:A:SER:N     | 20       | 0.26          |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H     | 8        | 0.26          |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H     | 19       | 0.26          |
| (2,2222) | 2:218:B:LEU:HD11 | 2:219:B:THR:H    | 8        | 0.25          |
| (2,2222) | 2:218:B:LEU:HD12 | 2:219:B:THR:H    | 8        | 0.25          |
| (2,2222) | 2:218:B:LEU:HD13 | 2:219:B:THR:H    | 8        | 0.25          |
| (2,2222) | 2:218:B:LEU:HD21 | 2:219:B:THR:H    | 8        | 0.25          |
| (2,2222) | 2:218:B:LEU:HD22 | 2:219:B:THR:H    | 8        | 0.25          |
| (2,2222) | 2:218:B:LEU:HD23 | 2:219:B:THR:H    | 8        | 0.25          |
| (2,2148) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HB3  | 12       | 0.25          |
| (2,2148) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HB3  | 12       | 0.25          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD11 | 9        | 0.25          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD12 | 9        | 0.25          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD13 | 9        | 0.25          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD21 | 9        | 0.25          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD22 | 9        | 0.25          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD23 | 9        | 0.25          |
| (2,2127) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HG   | 10       | 0.25          |
| (2,2127) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HG   | 10       | 0.25          |
| (2,2127) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HG   | 10       | 0.25          |
| (2,2127) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HG   | 10       | 0.25          |
| (2,2127) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HG   | 10       | 0.25          |
| (2,2127) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HG   | 10       | 0.25          |
| (2,2127) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HG   | 13       | 0.25          |
| (2,2127) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HG   | 13       | 0.25          |
| (2,2127) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HG   | 13       | 0.25          |
| (2,2127) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HG   | 13       | 0.25          |
| (2,2127) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HG   | 13       | 0.25          |
| (2,2127) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HG   | 13       | 0.25          |
| (2,2112) | 2:206:B:ARG:HD2  | 2:207:B:VAL:H    | 3        | 0.25          |
| (2,2112) | 2:206:B:ARG:HD3  | 2:207:B:VAL:H    | 3        | 0.25          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD11 | 4        | 0.25          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD12 | 4        | 0.25          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD13 | 4        | 0.25          |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD21 | 4        | 0.25          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1943) | 1:74:A:PHE:HD1  | 2:214:B:LEU:HD22 | 4        | 0.25          |
| (2,1943) | 1:74:A:PHE:HD1  | 2:214:B:LEU:HD23 | 4        | 0.25          |
| (2,1943) | 1:74:A:PHE:HD2  | 2:214:B:LEU:HD11 | 4        | 0.25          |
| (2,1943) | 1:74:A:PHE:HD2  | 2:214:B:LEU:HD12 | 4        | 0.25          |
| (2,1943) | 1:74:A:PHE:HD2  | 2:214:B:LEU:HD13 | 4        | 0.25          |
| (2,1943) | 1:74:A:PHE:HD2  | 2:214:B:LEU:HD21 | 4        | 0.25          |
| (2,1943) | 1:74:A:PHE:HD2  | 2:214:B:LEU:HD22 | 4        | 0.25          |
| (2,1943) | 1:74:A:PHE:HD2  | 2:214:B:LEU:HD23 | 4        | 0.25          |
| (2,1795) | 1:52:A:VAL:HG11 | 2:205:B:TRP:HZ2  | 11       | 0.25          |
| (2,1795) | 1:52:A:VAL:HG12 | 2:205:B:TRP:HZ2  | 11       | 0.25          |
| (2,1795) | 1:52:A:VAL:HG13 | 2:205:B:TRP:HZ2  | 11       | 0.25          |
| (2,1795) | 1:52:A:VAL:HG21 | 2:205:B:TRP:HZ2  | 11       | 0.25          |
| (2,1795) | 1:52:A:VAL:HG22 | 2:205:B:TRP:HZ2  | 11       | 0.25          |
| (2,1795) | 1:52:A:VAL:HG23 | 2:205:B:TRP:HZ2  | 11       | 0.25          |
| (2,1794) | 1:52:A:VAL:HG11 | 2:205:B:TRP:HZ3  | 13       | 0.25          |
| (2,1794) | 1:52:A:VAL:HG12 | 2:205:B:TRP:HZ3  | 13       | 0.25          |
| (2,1794) | 1:52:A:VAL:HG13 | 2:205:B:TRP:HZ3  | 13       | 0.25          |
| (2,1794) | 1:52:A:VAL:HG21 | 2:205:B:TRP:HZ3  | 13       | 0.25          |
| (2,1794) | 1:52:A:VAL:HG22 | 2:205:B:TRP:HZ3  | 13       | 0.25          |
| (2,1794) | 1:52:A:VAL:HG23 | 2:205:B:TRP:HZ3  | 13       | 0.25          |
| (2,1738) | 1:48:A:LEU:HD11 | 2:206:B:ARG:H    | 2        | 0.25          |
| (2,1738) | 1:48:A:LEU:HD12 | 2:206:B:ARG:H    | 2        | 0.25          |
| (2,1738) | 1:48:A:LEU:HD13 | 2:206:B:ARG:H    | 2        | 0.25          |
| (2,1738) | 1:48:A:LEU:HD21 | 2:206:B:ARG:H    | 2        | 0.25          |
| (2,1738) | 1:48:A:LEU:HD22 | 2:206:B:ARG:H    | 2        | 0.25          |
| (2,1738) | 1:48:A:LEU:HD23 | 2:206:B:ARG:H    | 2        | 0.25          |
| (2,1738) | 1:48:A:LEU:HD11 | 2:206:B:ARG:H    | 13       | 0.25          |
| (2,1738) | 1:48:A:LEU:HD12 | 2:206:B:ARG:H    | 13       | 0.25          |
| (2,1738) | 1:48:A:LEU:HD13 | 2:206:B:ARG:H    | 13       | 0.25          |
| (2,1738) | 1:48:A:LEU:HD21 | 2:206:B:ARG:H    | 13       | 0.25          |
| (2,1738) | 1:48:A:LEU:HD22 | 2:206:B:ARG:H    | 13       | 0.25          |
| (2,1738) | 1:48:A:LEU:HD23 | 2:206:B:ARG:H    | 13       | 0.25          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD11  | 12       | 0.25          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD12  | 12       | 0.25          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD13  | 12       | 0.25          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD21  | 12       | 0.25          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD22  | 12       | 0.25          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD23  | 12       | 0.25          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD11  | 12       | 0.25          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD12  | 12       | 0.25          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD13  | 12       | 0.25          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD21  | 12       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1619) | 1:35:A:GLN:HE22  | 1:38:A:LEU:HD22  | 12       | 0.25          |
| (2,1619) | 1:35:A:GLN:HE22  | 1:38:A:LEU:HD23  | 12       | 0.25          |
| (2,1545) | 1:28:A:MET:HE1   | 1:33:A:LYS:HG2   | 20       | 0.25          |
| (2,1545) | 1:28:A:MET:HE1   | 1:33:A:LYS:HG3   | 20       | 0.25          |
| (2,1545) | 1:28:A:MET:HE2   | 1:33:A:LYS:HG2   | 20       | 0.25          |
| (2,1545) | 1:28:A:MET:HE2   | 1:33:A:LYS:HG3   | 20       | 0.25          |
| (2,1545) | 1:28:A:MET:HE3   | 1:33:A:LYS:HG2   | 20       | 0.25          |
| (2,1545) | 1:28:A:MET:HE3   | 1:33:A:LYS:HG3   | 20       | 0.25          |
| (2,1475) | 1:73:A:ASP:HA    | 2:216:B:ILE:H    | 12       | 0.25          |
| (2,1464) | 2:205:B:TRP:HD1  | 2:221:B:GLU:H    | 15       | 0.25          |
| (2,1435) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H    | 4        | 0.25          |
| (2,1435) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H    | 4        | 0.25          |
| (2,1435) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H    | 4        | 0.25          |
| (2,1392) | 2:209:B:ARG:HD3  | 2:210:B:SER:H    | 14       | 0.25          |
| (2,1340) | 2:205:B:TRP:HE3  | 2:219:B:THR:H    | 6        | 0.25          |
| (2,1257) | 1:73:A:ASP:HA    | 2:215:B:LYS:HB2  | 17       | 0.25          |
| (2,1256) | 1:73:A:ASP:HA    | 2:215:B:LYS:HB3  | 11       | 0.25          |
| (2,1251) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HG   | 14       | 0.25          |
| (2,1237) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB2  | 5        | 0.25          |
| (2,1206) | 1:73:A:ASP:HA    | 2:215:B:LYS:HG3  | 18       | 0.25          |
| (2,1202) | 2:215:B:LYS:HG2  | 2:216:B:ILE:H    | 7        | 0.25          |
| (2,432)  | 1:53:A:HIS:HA    | 1:56:A:GLN:HB3   | 10       | 0.25          |
| (1,19)   | 1:83:A:ARG:O     | 1:87:A:ARG:N     | 16       | 0.25          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 9        | 0.25          |
| (2,2112) | 2:206:B:ARG:HD2  | 2:207:B:VAL:H    | 19       | 0.24          |
| (2,2112) | 2:206:B:ARG:HD3  | 2:207:B:VAL:H    | 19       | 0.24          |
| (2,1621) | 1:35:A:GLN:HE21  | 1:39:A:ASP:HB2   | 3        | 0.24          |
| (2,1621) | 1:35:A:GLN:HE21  | 1:39:A:ASP:HB3   | 3        | 0.24          |
| (2,1621) | 1:35:A:GLN:HE22  | 1:39:A:ASP:HB2   | 3        | 0.24          |
| (2,1621) | 1:35:A:GLN:HE22  | 1:39:A:ASP:HB3   | 3        | 0.24          |
| (2,1621) | 1:35:A:GLN:HE21  | 1:39:A:ASP:HB2   | 4        | 0.24          |
| (2,1621) | 1:35:A:GLN:HE21  | 1:39:A:ASP:HB3   | 4        | 0.24          |
| (2,1621) | 1:35:A:GLN:HE22  | 1:39:A:ASP:HB2   | 4        | 0.24          |
| (2,1621) | 1:35:A:GLN:HE22  | 1:39:A:ASP:HB3   | 4        | 0.24          |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB2  | 10       | 0.24          |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB3  | 10       | 0.24          |
| (2,1500) | 1:20:A:GLU:HB2   | 1:21:A:GLU:H     | 12       | 0.24          |
| (2,1500) | 1:20:A:GLU:HB3   | 1:21:A:GLU:H     | 12       | 0.24          |
| (2,1481) | 2:212:B:ASN:H    | 2:212:B:ASN:HD22 | 6        | 0.24          |
| (2,1464) | 2:205:B:TRP:HD1  | 2:221:B:GLU:H    | 3        | 0.24          |
| (2,1415) | 1:70:A:ILE:HB    | 2:218:B:LEU:H    | 14       | 0.24          |
| (2,1340) | 2:205:B:TRP:HE3  | 2:219:B:THR:H    | 5        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1300) | 1:73:A:ASP:HA    | 2:216:B:ILE:HG12 | 15       | 0.24          |
| (2,1251) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HG   | 16       | 0.24          |
| (2,1250) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HG   | 12       | 0.24          |
| (2,1250) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HG   | 12       | 0.24          |
| (2,1202) | 2:215:B:LYS:HG2  | 2:216:B:ILE:H    | 10       | 0.24          |
| (2,956)  | 1:21:A:GLU:HA    | 1:22:A:GLU:H     | 4        | 0.24          |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD11 | 5        | 0.24          |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD12 | 5        | 0.24          |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD13 | 5        | 0.24          |
| (2,23)   | 1:70:A:ILE:HD11  | 2:205:B:TRP:HH2  | 19       | 0.24          |
| (2,23)   | 1:70:A:ILE:HD12  | 2:205:B:TRP:HH2  | 19       | 0.24          |
| (2,23)   | 1:70:A:ILE:HD13  | 2:205:B:TRP:HH2  | 19       | 0.24          |
| (1,21)   | 1:87:A:ARG:O     | 1:91:A:SER:N     | 17       | 0.24          |
| (1,18)   | 1:53:A:HIS:O     | 1:57:A:SER:H     | 8        | 0.24          |
| (2,2210) | 2:217:B:ARG:H    | 2:218:B:LEU:HD11 | 18       | 0.23          |
| (2,2210) | 2:217:B:ARG:H    | 2:218:B:LEU:HD12 | 18       | 0.23          |
| (2,2210) | 2:217:B:ARG:H    | 2:218:B:LEU:HD13 | 18       | 0.23          |
| (2,2210) | 2:217:B:ARG:H    | 2:218:B:LEU:HD21 | 18       | 0.23          |
| (2,2210) | 2:217:B:ARG:H    | 2:218:B:LEU:HD22 | 18       | 0.23          |
| (2,2210) | 2:217:B:ARG:H    | 2:218:B:LEU:HD23 | 18       | 0.23          |
| (2,2200) | 2:214:B:LEU:HD11 | 2:215:B:LYS:HG3  | 11       | 0.23          |
| (2,2200) | 2:214:B:LEU:HD12 | 2:215:B:LYS:HG3  | 11       | 0.23          |
| (2,2200) | 2:214:B:LEU:HD13 | 2:215:B:LYS:HG3  | 11       | 0.23          |
| (2,2200) | 2:214:B:LEU:HD21 | 2:215:B:LYS:HG3  | 11       | 0.23          |
| (2,2200) | 2:214:B:LEU:HD22 | 2:215:B:LYS:HG3  | 11       | 0.23          |
| (2,2200) | 2:214:B:LEU:HD23 | 2:215:B:LYS:HG3  | 11       | 0.23          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD11 | 19       | 0.23          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD12 | 19       | 0.23          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD13 | 19       | 0.23          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD21 | 19       | 0.23          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD22 | 19       | 0.23          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD23 | 19       | 0.23          |
| (2,1738) | 1:48:A:LEU:HD11  | 2:206:B:ARG:H    | 7        | 0.23          |
| (2,1738) | 1:48:A:LEU:HD12  | 2:206:B:ARG:H    | 7        | 0.23          |
| (2,1738) | 1:48:A:LEU:HD13  | 2:206:B:ARG:H    | 7        | 0.23          |
| (2,1738) | 1:48:A:LEU:HD21  | 2:206:B:ARG:H    | 7        | 0.23          |
| (2,1738) | 1:48:A:LEU:HD22  | 2:206:B:ARG:H    | 7        | 0.23          |
| (2,1738) | 1:48:A:LEU:HD23  | 2:206:B:ARG:H    | 7        | 0.23          |
| (2,1738) | 1:48:A:LEU:HD11  | 2:206:B:ARG:H    | 16       | 0.23          |
| (2,1738) | 1:48:A:LEU:HD12  | 2:206:B:ARG:H    | 16       | 0.23          |
| (2,1738) | 1:48:A:LEU:HD13  | 2:206:B:ARG:H    | 16       | 0.23          |
| (2,1738) | 1:48:A:LEU:HD21  | 2:206:B:ARG:H    | 16       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1738) | 1:48:A:LEU:HD22  | 2:206:B:ARG:H    | 16       | 0.23          |
| (2,1738) | 1:48:A:LEU:HD23  | 2:206:B:ARG:H    | 16       | 0.23          |
| (2,1503) | 1:22:A:GLU:HB2   | 1:23:A:GLU:H     | 13       | 0.23          |
| (2,1503) | 1:22:A:GLU:HB3   | 1:23:A:GLU:H     | 13       | 0.23          |
| (2,1475) | 1:73:A:ASP:HA    | 2:216:B:ILE:H    | 1        | 0.23          |
| (2,1471) | 1:74:A:PHE:H     | 2:215:B:LYS:H    | 17       | 0.23          |
| (2,1451) | 1:71:A:GLU:HG3   | 2:218:B:LEU:H    | 3        | 0.23          |
| (2,1367) | 1:73:A:ASP:HA    | 2:215:B:LYS:H    | 20       | 0.23          |
| (2,1248) | 1:74:A:PHE:H     | 2:214:B:LEU:HD11 | 15       | 0.23          |
| (2,1248) | 1:74:A:PHE:H     | 2:214:B:LEU:HD12 | 15       | 0.23          |
| (2,1248) | 1:74:A:PHE:H     | 2:214:B:LEU:HD13 | 15       | 0.23          |
| (2,1161) | 1:68:A:ASP:HB2   | 2:220:B:ARG:HB2  | 17       | 0.23          |
| (2,801)  | 1:74:A:PHE:H     | 2:214:B:LEU:HB2  | 5        | 0.23          |
| (2,801)  | 1:74:A:PHE:H     | 2:214:B:LEU:HB2  | 12       | 0.23          |
| (2,650)  | 1:70:A:ILE:HB    | 2:205:B:TRP:HZ3  | 2        | 0.23          |
| (2,625)  | 1:72:A:ILE:HG21  | 2:216:B:ILE:HD11 | 15       | 0.23          |
| (2,625)  | 1:72:A:ILE:HG21  | 2:216:B:ILE:HD12 | 15       | 0.23          |
| (2,625)  | 1:72:A:ILE:HG21  | 2:216:B:ILE:HD13 | 15       | 0.23          |
| (2,625)  | 1:72:A:ILE:HG22  | 2:216:B:ILE:HD11 | 15       | 0.23          |
| (2,625)  | 1:72:A:ILE:HG22  | 2:216:B:ILE:HD12 | 15       | 0.23          |
| (2,625)  | 1:72:A:ILE:HG22  | 2:216:B:ILE:HD13 | 15       | 0.23          |
| (2,625)  | 1:72:A:ILE:HG23  | 2:216:B:ILE:HD11 | 15       | 0.23          |
| (2,625)  | 1:72:A:ILE:HG23  | 2:216:B:ILE:HD12 | 15       | 0.23          |
| (2,625)  | 1:72:A:ILE:HG23  | 2:216:B:ILE:HD13 | 15       | 0.23          |
| (2,613)  | 1:52:A:VAL:HG11  | 2:205:B:TRP:HZ2  | 6        | 0.23          |
| (2,613)  | 1:52:A:VAL:HG12  | 2:205:B:TRP:HZ2  | 6        | 0.23          |
| (2,613)  | 1:52:A:VAL:HG13  | 2:205:B:TRP:HZ2  | 6        | 0.23          |
| (2,103)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ2  | 4        | 0.23          |
| (2,103)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ2  | 4        | 0.23          |
| (2,103)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ2  | 4        | 0.23          |
| (1,3)    | 1:34:A:ARG:O     | 1:38:A:LEU:N     | 18       | 0.23          |
| (2,2222) | 2:218:B:LEU:HD11 | 2:219:B:THR:H    | 1        | 0.22          |
| (2,2222) | 2:218:B:LEU:HD12 | 2:219:B:THR:H    | 1        | 0.22          |
| (2,2222) | 2:218:B:LEU:HD13 | 2:219:B:THR:H    | 1        | 0.22          |
| (2,2222) | 2:218:B:LEU:HD21 | 2:219:B:THR:H    | 1        | 0.22          |
| (2,2222) | 2:218:B:LEU:HD22 | 2:219:B:THR:H    | 1        | 0.22          |
| (2,2222) | 2:218:B:LEU:HD23 | 2:219:B:THR:H    | 1        | 0.22          |
| (2,2216) | 2:217:B:ARG:HD2  | 2:219:B:THR:HB   | 11       | 0.22          |
| (2,2216) | 2:217:B:ARG:HD3  | 2:219:B:THR:HB   | 11       | 0.22          |
| (2,2199) | 2:214:B:LEU:HD11 | 2:215:B:LYS:H    | 4        | 0.22          |
| (2,2199) | 2:214:B:LEU:HD12 | 2:215:B:LYS:H    | 4        | 0.22          |
| (2,2199) | 2:214:B:LEU:HD13 | 2:215:B:LYS:H    | 4        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2199) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H    | 4        | 0.22          |
| (2,2199) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H    | 4        | 0.22          |
| (2,2199) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H    | 4        | 0.22          |
| (2,2187) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE2  | 7        | 0.22          |
| (2,2187) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HE3  | 7        | 0.22          |
| (2,2171) | 2:210:B:SER:HB2  | 2:215:B:LYS:HB2  | 2        | 0.22          |
| (2,2171) | 2:210:B:SER:HB3  | 2:215:B:LYS:HB2  | 2        | 0.22          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD11 | 14       | 0.22          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD12 | 14       | 0.22          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD13 | 14       | 0.22          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD21 | 14       | 0.22          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD22 | 14       | 0.22          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD23 | 14       | 0.22          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD11 | 12       | 0.22          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD12 | 12       | 0.22          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD13 | 12       | 0.22          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD21 | 12       | 0.22          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD22 | 12       | 0.22          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD23 | 12       | 0.22          |
| (2,2089) | 2:205:B:TRP:HB2  | 2:220:B:ARG:HB2  | 8        | 0.22          |
| (2,2089) | 2:205:B:TRP:HB2  | 2:220:B:ARG:HB3  | 8        | 0.22          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD11 | 5        | 0.22          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD12 | 5        | 0.22          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD13 | 5        | 0.22          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD21 | 5        | 0.22          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD22 | 5        | 0.22          |
| (2,1954) | 1:75:A:GLU:HG2   | 2:214:B:LEU:HD23 | 5        | 0.22          |
| (2,1930) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG2  | 14       | 0.22          |
| (2,1930) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG2  | 14       | 0.22          |
| (2,1805) | 1:54:A:ILE:HG21  | 1:84:A:GLU:HB2   | 6        | 0.22          |
| (2,1805) | 1:54:A:ILE:HG21  | 1:84:A:GLU:HB3   | 6        | 0.22          |
| (2,1805) | 1:54:A:ILE:HG22  | 1:84:A:GLU:HB2   | 6        | 0.22          |
| (2,1805) | 1:54:A:ILE:HG22  | 1:84:A:GLU:HB3   | 6        | 0.22          |
| (2,1805) | 1:54:A:ILE:HG23  | 1:84:A:GLU:HB2   | 6        | 0.22          |
| (2,1805) | 1:54:A:ILE:HG23  | 1:84:A:GLU:HB3   | 6        | 0.22          |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB2  | 4        | 0.22          |
| (2,1602) | 1:34:A:ARG:HG3   | 2:213:B:PRO:HB3  | 4        | 0.22          |
| (2,1486) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB3  | 3        | 0.22          |
| (2,1464) | 2:205:B:TRP:HD1  | 2:221:B:GLU:H    | 12       | 0.22          |
| (2,1464) | 2:205:B:TRP:HD1  | 2:221:B:GLU:H    | 20       | 0.22          |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG   | 2        | 0.22          |
| (2,1383) | 2:206:B:ARG:H    | 2:220:B:ARG:HA   | 16       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1383) | 2:206:B:ARG:H    | 2:220:B:ARG:HA   | 19       | 0.22          |
| (2,1288) | 1:52:A:VAL:HG21  | 2:218:B:LEU:HG   | 19       | 0.22          |
| (2,1288) | 1:52:A:VAL:HG22  | 2:218:B:LEU:HG   | 19       | 0.22          |
| (2,1288) | 1:52:A:VAL:HG23  | 2:218:B:LEU:HG   | 19       | 0.22          |
| (2,1262) | 1:69:A:GLU:H     | 2:219:B:THR:HA   | 9        | 0.22          |
| (2,1257) | 1:73:A:ASP:HA    | 2:215:B:LYS:HB2  | 18       | 0.22          |
| (2,1251) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HG   | 9        | 0.22          |
| (2,990)  | 1:69:A:GLU:H     | 2:205:B:TRP:HZ3  | 15       | 0.22          |
| (2,634)  | 1:70:A:ILE:H     | 1:71:A:GLU:HG3   | 8        | 0.22          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 9        | 0.22          |
| (1,12)   | 1:50:A:ARG:O     | 1:54:A:ILE:H     | 4        | 0.22          |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H     | 13       | 0.22          |
| (1,2)    | 1:33:A:LYS:O     | 1:37:A:SER:H     | 15       | 0.22          |
| (2,2171) | 2:210:B:SER:HB2  | 2:215:B:LYS:HB2  | 4        | 0.21          |
| (2,2171) | 2:210:B:SER:HB3  | 2:215:B:LYS:HB2  | 4        | 0.21          |
| (2,2141) | 2:208:B:GLN:HB2  | 2:219:B:THR:H    | 10       | 0.21          |
| (2,2141) | 2:208:B:GLN:HB3  | 2:219:B:THR:H    | 10       | 0.21          |
| (2,2119) | 2:207:B:VAL:HG11 | 2:208:B:GLN:H    | 8        | 0.21          |
| (2,2119) | 2:207:B:VAL:HG12 | 2:208:B:GLN:H    | 8        | 0.21          |
| (2,2119) | 2:207:B:VAL:HG13 | 2:208:B:GLN:H    | 8        | 0.21          |
| (2,2119) | 2:207:B:VAL:HG21 | 2:208:B:GLN:H    | 8        | 0.21          |
| (2,2119) | 2:207:B:VAL:HG22 | 2:208:B:GLN:H    | 8        | 0.21          |
| (2,2119) | 2:207:B:VAL:HG23 | 2:208:B:GLN:H    | 8        | 0.21          |
| (2,2119) | 2:207:B:VAL:HG11 | 2:208:B:GLN:H    | 18       | 0.21          |
| (2,2119) | 2:207:B:VAL:HG12 | 2:208:B:GLN:H    | 18       | 0.21          |
| (2,2119) | 2:207:B:VAL:HG13 | 2:208:B:GLN:H    | 18       | 0.21          |
| (2,2119) | 2:207:B:VAL:HG21 | 2:208:B:GLN:H    | 18       | 0.21          |
| (2,2119) | 2:207:B:VAL:HG22 | 2:208:B:GLN:H    | 18       | 0.21          |
| (2,2119) | 2:207:B:VAL:HG23 | 2:208:B:GLN:H    | 18       | 0.21          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD11 | 15       | 0.21          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD12 | 15       | 0.21          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD13 | 15       | 0.21          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD21 | 15       | 0.21          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD22 | 15       | 0.21          |
| (2,2093) | 2:205:B:TRP:HE3  | 2:218:B:LEU:HD23 | 15       | 0.21          |
| (2,2068) | 1:95:A:LYS:H     | 1:96:A:LYS:HG2   | 16       | 0.21          |
| (2,2068) | 1:95:A:LYS:H     | 1:96:A:LYS:HG3   | 16       | 0.21          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD11 | 16       | 0.21          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD12 | 16       | 0.21          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD13 | 16       | 0.21          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD21 | 16       | 0.21          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD22 | 16       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD23 | 16       | 0.21          |
| (2,1503) | 1:22:A:GLU:HB2   | 1:23:A:GLU:H     | 18       | 0.21          |
| (2,1503) | 1:22:A:GLU:HB3   | 1:23:A:GLU:H     | 18       | 0.21          |
| (2,1503) | 1:22:A:GLU:HB2   | 1:23:A:GLU:H     | 19       | 0.21          |
| (2,1503) | 1:22:A:GLU:HB3   | 1:23:A:GLU:H     | 19       | 0.21          |
| (2,1500) | 1:20:A:GLU:HB2   | 1:21:A:GLU:H     | 7        | 0.21          |
| (2,1500) | 1:20:A:GLU:HB3   | 1:21:A:GLU:H     | 7        | 0.21          |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG   | 12       | 0.21          |
| (2,1416) | 2:215:B:LYS:H    | 2:215:B:LYS:HB2  | 2        | 0.21          |
| (2,1286) | 1:74:A:PHE:H     | 2:215:B:LYS:HG3  | 7        | 0.21          |
| (2,1208) | 2:215:B:LYS:HA   | 2:215:B:LYS:HD2  | 18       | 0.21          |
| (2,1202) | 2:215:B:LYS:HG2  | 2:216:B:ILE:H    | 17       | 0.21          |
| (2,1174) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HB2  | 2        | 0.21          |
| (2,801)  | 1:74:A:PHE:H     | 2:214:B:LEU:HB2  | 16       | 0.21          |
| (2,633)  | 1:71:A:GLU:HG3   | 2:217:B:ARG:HG2  | 8        | 0.21          |
| (2,553)  | 1:27:A:PRO:HA    | 1:79:A:PRO:HB3   | 17       | 0.21          |
| (2,152)  | 1:34:A:ARG:HA    | 2:214:B:LEU:HG   | 18       | 0.21          |
| (2,103)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HZ2  | 11       | 0.21          |
| (2,103)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HZ2  | 11       | 0.21          |
| (2,103)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HZ2  | 11       | 0.21          |
| (2,5)    | 1:36:A:LEU:HG    | 1:74:A:PHE:HZ    | 5        | 0.21          |
| (1,22)   | 1:87:A:ARG:O     | 1:91:A:SER:H     | 13       | 0.21          |
| (1,3)    | 1:34:A:ARG:O     | 1:38:A:LEU:N     | 10       | 0.21          |
| (2,2199) | 2:214:B:LEU:HD11 | 2:215:B:LYS:H    | 14       | 0.2           |
| (2,2199) | 2:214:B:LEU:HD12 | 2:215:B:LYS:H    | 14       | 0.2           |
| (2,2199) | 2:214:B:LEU:HD13 | 2:215:B:LYS:H    | 14       | 0.2           |
| (2,2199) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H    | 14       | 0.2           |
| (2,2199) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H    | 14       | 0.2           |
| (2,2199) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H    | 14       | 0.2           |
| (2,2032) | 1:87:A:ARG:HD2   | 1:88:A:TYR:HD1   | 19       | 0.2           |
| (2,2032) | 1:87:A:ARG:HD2   | 1:88:A:TYR:HD2   | 19       | 0.2           |
| (2,2032) | 1:87:A:ARG:HD3   | 1:88:A:TYR:HD1   | 19       | 0.2           |
| (2,2032) | 1:87:A:ARG:HD3   | 1:88:A:TYR:HD2   | 19       | 0.2           |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD11 | 14       | 0.2           |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD12 | 14       | 0.2           |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD13 | 14       | 0.2           |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD21 | 14       | 0.2           |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD22 | 14       | 0.2           |
| (2,1943) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HD23 | 14       | 0.2           |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD11 | 14       | 0.2           |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD12 | 14       | 0.2           |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD13 | 14       | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD21 | 14       | 0.2           |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD22 | 14       | 0.2           |
| (2,1943) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HD23 | 14       | 0.2           |
| (2,1865) | 1:62:A:LEU:HB2   | 1:65:A:SER:HB2   | 1        | 0.2           |
| (2,1865) | 1:62:A:LEU:HB2   | 1:65:A:SER:HB3   | 1        | 0.2           |
| (2,1865) | 1:62:A:LEU:HB3   | 1:65:A:SER:HB2   | 1        | 0.2           |
| (2,1865) | 1:62:A:LEU:HB3   | 1:65:A:SER:HB3   | 1        | 0.2           |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD11 | 5        | 0.2           |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD12 | 5        | 0.2           |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD13 | 5        | 0.2           |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD21 | 5        | 0.2           |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD22 | 5        | 0.2           |
| (2,1654) | 1:37:A:SER:HB2   | 2:214:B:LEU:HD23 | 5        | 0.2           |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD11 | 5        | 0.2           |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD12 | 5        | 0.2           |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD13 | 5        | 0.2           |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD21 | 5        | 0.2           |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD22 | 5        | 0.2           |
| (2,1597) | 1:34:A:ARG:HA    | 2:214:B:LEU:HD23 | 5        | 0.2           |
| (2,1440) | 2:214:B:LEU:HD11 | 2:215:B:LYS:H    | 20       | 0.2           |
| (2,1440) | 2:214:B:LEU:HD12 | 2:215:B:LYS:H    | 20       | 0.2           |
| (2,1440) | 2:214:B:LEU:HD13 | 2:215:B:LYS:H    | 20       | 0.2           |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG   | 4        | 0.2           |
| (2,1356) | 2:205:B:TRP:HE3  | 2:220:B:ARG:H    | 11       | 0.2           |
| (2,1353) | 1:74:A:PHE:HD1   | 2:215:B:LYS:H    | 3        | 0.2           |
| (2,1353) | 1:74:A:PHE:HD2   | 2:215:B:LYS:H    | 3        | 0.2           |
| (2,1250) | 1:74:A:PHE:HD1   | 2:214:B:LEU:HG   | 19       | 0.2           |
| (2,1250) | 1:74:A:PHE:HD2   | 2:214:B:LEU:HG   | 19       | 0.2           |
| (2,1238) | 2:215:B:LYS:HB3  | 2:215:B:LYS:HE3  | 17       | 0.2           |
| (2,1238) | 2:215:B:LYS:HB3  | 2:215:B:LYS:HE3  | 18       | 0.2           |
| (2,1146) | 2:219:B:THR:H    | 2:219:B:THR:HG21 | 7        | 0.2           |
| (2,1146) | 2:219:B:THR:H    | 2:219:B:THR:HG22 | 7        | 0.2           |
| (2,1146) | 2:219:B:THR:H    | 2:219:B:THR:HG23 | 7        | 0.2           |
| (2,1102) | 1:75:A:GLU:H     | 2:215:B:LYS:HA   | 13       | 0.2           |
| (2,720)  | 1:74:A:PHE:H     | 2:215:B:LYS:HG2  | 20       | 0.2           |
| (2,436)  | 1:57:A:SER:HA    | 1:60:A:PRO:HA    | 18       | 0.2           |
| (2,432)  | 1:53:A:HIS:HA    | 1:56:A:GLN:HB3   | 11       | 0.2           |
| (2,101)  | 1:52:A:VAL:HG21  | 2:205:B:TRP:HH2  | 16       | 0.2           |
| (2,101)  | 1:52:A:VAL:HG22  | 2:205:B:TRP:HH2  | 16       | 0.2           |
| (2,101)  | 1:52:A:VAL:HG23  | 2:205:B:TRP:HH2  | 16       | 0.2           |
| (1,17)   | 1:53:A:HIS:O     | 1:57:A:SER:N     | 10       | 0.2           |
| (1,12)   | 1:50:A:ARG:O     | 1:54:A:ILE:H     | 11       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,12)   | 1:50:A:ARG:O    | 1:54:A:ILE:H    | 13       | 0.2           |
| (2,2165) | 2:209:B:ARG:HD2 | 2:210:B:SER:H   | 20       | 0.19          |
| (2,2165) | 2:209:B:ARG:HD3 | 2:210:B:SER:H   | 20       | 0.19          |
| (2,2141) | 2:208:B:GLN:HB2 | 2:219:B:THR:H   | 19       | 0.19          |
| (2,2141) | 2:208:B:GLN:HB3 | 2:219:B:THR:H   | 19       | 0.19          |
| (2,2140) | 2:208:B:GLN:HB2 | 2:217:B:ARG:HD2 | 2        | 0.19          |
| (2,2140) | 2:208:B:GLN:HB2 | 2:217:B:ARG:HD3 | 2        | 0.19          |
| (2,2140) | 2:208:B:GLN:HB3 | 2:217:B:ARG:HD2 | 2        | 0.19          |
| (2,2140) | 2:208:B:GLN:HB3 | 2:217:B:ARG:HD3 | 2        | 0.19          |
| (2,2140) | 2:208:B:GLN:HB2 | 2:217:B:ARG:HD2 | 5        | 0.19          |
| (2,2140) | 2:208:B:GLN:HB2 | 2:217:B:ARG:HD3 | 5        | 0.19          |
| (2,2140) | 2:208:B:GLN:HB3 | 2:217:B:ARG:HD2 | 5        | 0.19          |
| (2,2140) | 2:208:B:GLN:HB3 | 2:217:B:ARG:HD3 | 5        | 0.19          |
| (2,2084) | 2:205:B:TRP:H   | 2:220:B:ARG:HG2 | 8        | 0.19          |
| (2,2084) | 2:205:B:TRP:H   | 2:220:B:ARG:HG3 | 8        | 0.19          |
| (2,2050) | 1:90:A:LYS:HA   | 1:90:A:LYS:HD2  | 11       | 0.19          |
| (2,2050) | 1:90:A:LYS:HA   | 1:90:A:LYS:HD3  | 11       | 0.19          |
| (2,2043) | 1:89:A:VAL:HG11 | 1:90:A:LYS:HG2  | 1        | 0.19          |
| (2,2043) | 1:89:A:VAL:HG11 | 1:90:A:LYS:HG3  | 1        | 0.19          |
| (2,2043) | 1:89:A:VAL:HG12 | 1:90:A:LYS:HG2  | 1        | 0.19          |
| (2,2043) | 1:89:A:VAL:HG12 | 1:90:A:LYS:HG3  | 1        | 0.19          |
| (2,2043) | 1:89:A:VAL:HG13 | 1:90:A:LYS:HG2  | 1        | 0.19          |
| (2,2043) | 1:89:A:VAL:HG13 | 1:90:A:LYS:HG3  | 1        | 0.19          |
| (2,2043) | 1:89:A:VAL:HG21 | 1:90:A:LYS:HG2  | 1        | 0.19          |
| (2,2043) | 1:89:A:VAL:HG21 | 1:90:A:LYS:HG3  | 1        | 0.19          |
| (2,2043) | 1:89:A:VAL:HG22 | 1:90:A:LYS:HG2  | 1        | 0.19          |
| (2,2043) | 1:89:A:VAL:HG22 | 1:90:A:LYS:HG3  | 1        | 0.19          |
| (2,2043) | 1:89:A:VAL:HG23 | 1:90:A:LYS:HG2  | 1        | 0.19          |
| (2,2043) | 1:89:A:VAL:HG23 | 1:90:A:LYS:HG3  | 1        | 0.19          |
| (2,1965) | 1:77:A:LEU:HD11 | 1:78:A:LYS:HB2  | 19       | 0.19          |
| (2,1965) | 1:77:A:LEU:HD12 | 1:78:A:LYS:HB2  | 19       | 0.19          |
| (2,1965) | 1:77:A:LEU:HD13 | 1:78:A:LYS:HB2  | 19       | 0.19          |
| (2,1965) | 1:77:A:LEU:HD21 | 1:78:A:LYS:HB2  | 19       | 0.19          |
| (2,1965) | 1:77:A:LEU:HD22 | 1:78:A:LYS:HB2  | 19       | 0.19          |
| (2,1965) | 1:77:A:LEU:HD23 | 1:78:A:LYS:HB2  | 19       | 0.19          |
| (2,1865) | 1:62:A:LEU:HB2  | 1:65:A:SER:HB2  | 2        | 0.19          |
| (2,1865) | 1:62:A:LEU:HB2  | 1:65:A:SER:HB3  | 2        | 0.19          |
| (2,1865) | 1:62:A:LEU:HB3  | 1:65:A:SER:HB2  | 2        | 0.19          |
| (2,1865) | 1:62:A:LEU:HB3  | 1:65:A:SER:HB3  | 2        | 0.19          |
| (2,1740) | 1:48:A:LEU:HD11 | 2:206:B:ARG:HB2 | 4        | 0.19          |
| (2,1740) | 1:48:A:LEU:HD11 | 2:206:B:ARG:HB3 | 4        | 0.19          |
| (2,1740) | 1:48:A:LEU:HD12 | 2:206:B:ARG:HB2 | 4        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1740) | 1:48:A:LEU:HD12 | 2:206:B:ARG:HB3 | 4        | 0.19          |
| (2,1740) | 1:48:A:LEU:HD13 | 2:206:B:ARG:HB2 | 4        | 0.19          |
| (2,1740) | 1:48:A:LEU:HD13 | 2:206:B:ARG:HB3 | 4        | 0.19          |
| (2,1740) | 1:48:A:LEU:HD21 | 2:206:B:ARG:HB2 | 4        | 0.19          |
| (2,1740) | 1:48:A:LEU:HD21 | 2:206:B:ARG:HB3 | 4        | 0.19          |
| (2,1740) | 1:48:A:LEU:HD22 | 2:206:B:ARG:HB2 | 4        | 0.19          |
| (2,1740) | 1:48:A:LEU:HD22 | 2:206:B:ARG:HB3 | 4        | 0.19          |
| (2,1740) | 1:48:A:LEU:HD23 | 2:206:B:ARG:HB2 | 4        | 0.19          |
| (2,1740) | 1:48:A:LEU:HD23 | 2:206:B:ARG:HB3 | 4        | 0.19          |
| (2,1737) | 1:48:A:LEU:HD11 | 2:205:B:TRP:HZ2 | 16       | 0.19          |
| (2,1737) | 1:48:A:LEU:HD12 | 2:205:B:TRP:HZ2 | 16       | 0.19          |
| (2,1737) | 1:48:A:LEU:HD13 | 2:205:B:TRP:HZ2 | 16       | 0.19          |
| (2,1737) | 1:48:A:LEU:HD21 | 2:205:B:TRP:HZ2 | 16       | 0.19          |
| (2,1737) | 1:48:A:LEU:HD22 | 2:205:B:TRP:HZ2 | 16       | 0.19          |
| (2,1737) | 1:48:A:LEU:HD23 | 2:205:B:TRP:HZ2 | 16       | 0.19          |
| (2,1736) | 1:48:A:LEU:HD11 | 2:205:B:TRP:H   | 5        | 0.19          |
| (2,1736) | 1:48:A:LEU:HD12 | 2:205:B:TRP:H   | 5        | 0.19          |
| (2,1736) | 1:48:A:LEU:HD13 | 2:205:B:TRP:H   | 5        | 0.19          |
| (2,1736) | 1:48:A:LEU:HD21 | 2:205:B:TRP:H   | 5        | 0.19          |
| (2,1736) | 1:48:A:LEU:HD22 | 2:205:B:TRP:H   | 5        | 0.19          |
| (2,1736) | 1:48:A:LEU:HD23 | 2:205:B:TRP:H   | 5        | 0.19          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD11 | 1        | 0.19          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD12 | 1        | 0.19          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD13 | 1        | 0.19          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD21 | 1        | 0.19          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD22 | 1        | 0.19          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD23 | 1        | 0.19          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD11 | 1        | 0.19          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD12 | 1        | 0.19          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD13 | 1        | 0.19          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD21 | 1        | 0.19          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD22 | 1        | 0.19          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD23 | 1        | 0.19          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD11 | 17       | 0.19          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD12 | 17       | 0.19          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD13 | 17       | 0.19          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD21 | 17       | 0.19          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD22 | 17       | 0.19          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD23 | 17       | 0.19          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD11 | 17       | 0.19          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD12 | 17       | 0.19          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD13 | 17       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1619) | 1:35:A:GLN:HE22  | 1:38:A:LEU:HD21  | 17       | 0.19          |
| (2,1619) | 1:35:A:GLN:HE22  | 1:38:A:LEU:HD22  | 17       | 0.19          |
| (2,1619) | 1:35:A:GLN:HE22  | 1:38:A:LEU:HD23  | 17       | 0.19          |
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD11  | 16       | 0.19          |
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD12  | 16       | 0.19          |
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD13  | 16       | 0.19          |
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD21  | 16       | 0.19          |
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD22  | 16       | 0.19          |
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD23  | 16       | 0.19          |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD11  | 16       | 0.19          |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD12  | 16       | 0.19          |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD13  | 16       | 0.19          |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD21  | 16       | 0.19          |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD22  | 16       | 0.19          |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD23  | 16       | 0.19          |
| (2,1478) | 2:208:B:GLN:HE21 | 2:219:B:THR:HG21 | 19       | 0.19          |
| (2,1478) | 2:208:B:GLN:HE21 | 2:219:B:THR:HG22 | 19       | 0.19          |
| (2,1478) | 2:208:B:GLN:HE21 | 2:219:B:THR:HG23 | 19       | 0.19          |
| (2,1293) | 1:69:A:GLU:HG3   | 2:219:B:THR:HB   | 19       | 0.19          |
| (2,1288) | 1:52:A:VAL:HG21  | 2:218:B:LEU:HG   | 7        | 0.19          |
| (2,1288) | 1:52:A:VAL:HG22  | 2:218:B:LEU:HG   | 7        | 0.19          |
| (2,1288) | 1:52:A:VAL:HG23  | 2:218:B:LEU:HG   | 7        | 0.19          |
| (2,1102) | 1:75:A:GLU:H     | 2:215:B:LYS:HA   | 10       | 0.19          |
| (2,802)  | 1:74:A:PHE:H     | 2:214:B:LEU:HB3  | 3        | 0.19          |
| (2,799)  | 1:22:A:GLU:HB2   | 1:23:A:GLU:H     | 8        | 0.19          |
| (2,636)  | 1:69:A:GLU:HA    | 2:219:B:THR:HG21 | 11       | 0.19          |
| (2,636)  | 1:69:A:GLU:HA    | 2:219:B:THR:HG22 | 11       | 0.19          |
| (2,636)  | 1:69:A:GLU:HA    | 2:219:B:THR:HG23 | 11       | 0.19          |
| (2,468)  | 1:69:A:GLU:HG2   | 1:70:A:ILE:H     | 8        | 0.19          |
| (2,152)  | 1:34:A:ARG:HA    | 2:214:B:LEU:HG   | 8        | 0.19          |
| (2,14)   | 1:70:A:ILE:HD11  | 2:205:B:TRP:HZ3  | 17       | 0.19          |
| (2,14)   | 1:70:A:ILE:HD12  | 2:205:B:TRP:HZ3  | 17       | 0.19          |
| (2,14)   | 1:70:A:ILE:HD13  | 2:205:B:TRP:HZ3  | 17       | 0.19          |
| (1,21)   | 1:87:A:ARG:O     | 1:91:A:SER:N     | 10       | 0.19          |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 12       | 0.19          |
| (1,9)    | 1:49:A:GLY:O     | 1:53:A:HIS:N     | 7        | 0.19          |
| (2,2121) | 2:207:B:VAL:HG11 | 2:216:B:ILE:HB   | 12       | 0.18          |
| (2,2121) | 2:207:B:VAL:HG12 | 2:216:B:ILE:HB   | 12       | 0.18          |
| (2,2121) | 2:207:B:VAL:HG13 | 2:216:B:ILE:HB   | 12       | 0.18          |
| (2,2121) | 2:207:B:VAL:HG21 | 2:216:B:ILE:HB   | 12       | 0.18          |
| (2,2121) | 2:207:B:VAL:HG22 | 2:216:B:ILE:HB   | 12       | 0.18          |
| (2,2121) | 2:207:B:VAL:HG23 | 2:216:B:ILE:HB   | 12       | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,2100) | 2:206:B:ARG:H   | 2:206:B:ARG:HD2  | 11       | 0.18          |
| (2,2100) | 2:206:B:ARG:H   | 2:206:B:ARG:HD3  | 11       | 0.18          |
| (2,2071) | 1:95:A:LYS:HB2  | 1:96:A:LYS:HG2   | 1        | 0.18          |
| (2,2071) | 1:95:A:LYS:HB2  | 1:96:A:LYS:HG3   | 1        | 0.18          |
| (2,2071) | 1:95:A:LYS:HB3  | 1:96:A:LYS:HG2   | 1        | 0.18          |
| (2,2071) | 1:95:A:LYS:HB3  | 1:96:A:LYS:HG3   | 1        | 0.18          |
| (2,2031) | 1:87:A:ARG:HD2  | 1:88:A:TYR:HA    | 15       | 0.18          |
| (2,2031) | 1:87:A:ARG:HD3  | 1:88:A:TYR:HA    | 15       | 0.18          |
| (2,1911) | 1:69:A:GLU:HG2  | 2:220:B:ARG:H    | 14       | 0.18          |
| (2,1911) | 1:69:A:GLU:HG3  | 2:220:B:ARG:H    | 14       | 0.18          |
| (2,1731) | 1:48:A:LEU:HB2  | 2:218:B:LEU:HD11 | 8        | 0.18          |
| (2,1731) | 1:48:A:LEU:HB2  | 2:218:B:LEU:HD12 | 8        | 0.18          |
| (2,1731) | 1:48:A:LEU:HB2  | 2:218:B:LEU:HD13 | 8        | 0.18          |
| (2,1731) | 1:48:A:LEU:HB2  | 2:218:B:LEU:HD21 | 8        | 0.18          |
| (2,1731) | 1:48:A:LEU:HB2  | 2:218:B:LEU:HD22 | 8        | 0.18          |
| (2,1731) | 1:48:A:LEU:HB2  | 2:218:B:LEU:HD23 | 8        | 0.18          |
| (2,1731) | 1:48:A:LEU:HB3  | 2:218:B:LEU:HD11 | 8        | 0.18          |
| (2,1731) | 1:48:A:LEU:HB3  | 2:218:B:LEU:HD12 | 8        | 0.18          |
| (2,1731) | 1:48:A:LEU:HB3  | 2:218:B:LEU:HD13 | 8        | 0.18          |
| (2,1731) | 1:48:A:LEU:HB3  | 2:218:B:LEU:HD21 | 8        | 0.18          |
| (2,1731) | 1:48:A:LEU:HB3  | 2:218:B:LEU:HD22 | 8        | 0.18          |
| (2,1731) | 1:48:A:LEU:HB3  | 2:218:B:LEU:HD23 | 8        | 0.18          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB2   | 10       | 0.18          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB3   | 10       | 0.18          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB2   | 10       | 0.18          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB3   | 10       | 0.18          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD11  | 16       | 0.18          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD12  | 16       | 0.18          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD13  | 16       | 0.18          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD21  | 16       | 0.18          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD22  | 16       | 0.18          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD23  | 16       | 0.18          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD11  | 16       | 0.18          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD12  | 16       | 0.18          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD13  | 16       | 0.18          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD21  | 16       | 0.18          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD22  | 16       | 0.18          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD23  | 16       | 0.18          |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD11  | 9        | 0.18          |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD12  | 9        | 0.18          |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD13  | 9        | 0.18          |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD21  | 9        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD22  | 9        | 0.18          |
| (2,1604) | 1:34:A:ARG:HD2   | 1:38:A:LEU:HD23  | 9        | 0.18          |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD11  | 9        | 0.18          |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD12  | 9        | 0.18          |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD13  | 9        | 0.18          |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD21  | 9        | 0.18          |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD22  | 9        | 0.18          |
| (2,1604) | 1:34:A:ARG:HD3   | 1:38:A:LEU:HD23  | 9        | 0.18          |
| (2,1481) | 2:212:B:ASN:H    | 2:212:B:ASN:HD22 | 12       | 0.18          |
| (2,1475) | 1:73:A:ASP:HA    | 2:216:B:ILE:H    | 4        | 0.18          |
| (2,1438) | 2:203:B:LEU:HD11 | 2:204:B:THR:H    | 20       | 0.18          |
| (2,1438) | 2:203:B:LEU:HD12 | 2:204:B:THR:H    | 20       | 0.18          |
| (2,1438) | 2:203:B:LEU:HD13 | 2:204:B:THR:H    | 20       | 0.18          |
| (2,1406) | 2:214:B:LEU:HB2  | 2:215:B:LYS:H    | 12       | 0.18          |
| (2,1396) | 2:205:B:TRP:HB2  | 2:206:B:ARG:H    | 6        | 0.18          |
| (2,1386) | 2:204:B:THR:HB   | 2:205:B:TRP:H    | 11       | 0.18          |
| (2,1208) | 2:215:B:LYS:HA   | 2:215:B:LYS:HD2  | 17       | 0.18          |
| (2,1131) | 1:72:A:ILE:H     | 2:217:B:ARG:HB2  | 20       | 0.18          |
| (2,965)  | 1:74:A:PHE:H     | 2:214:B:LEU:HA   | 14       | 0.18          |
| (2,799)  | 1:22:A:GLU:HB2   | 1:23:A:GLU:H     | 20       | 0.18          |
| (2,553)  | 1:27:A:PRO:HA    | 1:79:A:PRO:HB3   | 3        | 0.18          |
| (2,553)  | 1:27:A:PRO:HA    | 1:79:A:PRO:HB3   | 18       | 0.18          |
| (2,410)  | 1:50:A:ARG:HG2   | 1:54:A:ILE:HD11  | 7        | 0.18          |
| (2,410)  | 1:50:A:ARG:HG2   | 1:54:A:ILE:HD12  | 7        | 0.18          |
| (2,410)  | 1:50:A:ARG:HG2   | 1:54:A:ILE:HD13  | 7        | 0.18          |
| (2,189)  | 1:70:A:ILE:HG12  | 2:205:B:TRP:HH2  | 1        | 0.18          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD21  | 4        | 0.18          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD22  | 4        | 0.18          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD23  | 4        | 0.18          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD21  | 4        | 0.18          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD22  | 4        | 0.18          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD23  | 4        | 0.18          |
| (1,18)   | 1:53:A:HIS:O     | 1:57:A:SER:H     | 20       | 0.18          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 12       | 0.18          |
| (1,13)   | 1:51:A:VAL:O     | 1:55:A:ILE:N     | 3        | 0.18          |
| (1,9)    | 1:49:A:GLY:O     | 1:53:A:HIS:N     | 2        | 0.18          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD11 | 16       | 0.17          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD12 | 16       | 0.17          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD13 | 16       | 0.17          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD21 | 16       | 0.17          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD22 | 16       | 0.17          |
| (2,2132) | 2:208:B:GLN:H    | 2:218:B:LEU:HD23 | 16       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2123) | 2:207:B:VAL:HG11 | 2:217:B:ARG:HA   | 18       | 0.17          |
| (2,2123) | 2:207:B:VAL:HG12 | 2:217:B:ARG:HA   | 18       | 0.17          |
| (2,2123) | 2:207:B:VAL:HG13 | 2:217:B:ARG:HA   | 18       | 0.17          |
| (2,2123) | 2:207:B:VAL:HG21 | 2:217:B:ARG:HA   | 18       | 0.17          |
| (2,2123) | 2:207:B:VAL:HG22 | 2:217:B:ARG:HA   | 18       | 0.17          |
| (2,2123) | 2:207:B:VAL:HG23 | 2:217:B:ARG:HA   | 18       | 0.17          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD11 | 11       | 0.17          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD12 | 11       | 0.17          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD13 | 11       | 0.17          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD21 | 11       | 0.17          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD22 | 11       | 0.17          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD23 | 11       | 0.17          |
| (2,2089) | 2:205:B:TRP:HB2  | 2:220:B:ARG:HB2  | 1        | 0.17          |
| (2,2089) | 2:205:B:TRP:HB2  | 2:220:B:ARG:HB3  | 1        | 0.17          |
| (2,2086) | 2:205:B:TRP:HA   | 2:220:B:ARG:HB2  | 10       | 0.17          |
| (2,2086) | 2:205:B:TRP:HA   | 2:220:B:ARG:HB3  | 10       | 0.17          |
| (2,2084) | 2:205:B:TRP:H    | 2:220:B:ARG:HG2  | 5        | 0.17          |
| (2,2084) | 2:205:B:TRP:H    | 2:220:B:ARG:HG3  | 5        | 0.17          |
| (2,2081) | 2:203:B:LEU:HD11 | 2:204:B:THR:H    | 15       | 0.17          |
| (2,2081) | 2:203:B:LEU:HD12 | 2:204:B:THR:H    | 15       | 0.17          |
| (2,2081) | 2:203:B:LEU:HD13 | 2:204:B:THR:H    | 15       | 0.17          |
| (2,2081) | 2:203:B:LEU:HD21 | 2:204:B:THR:H    | 15       | 0.17          |
| (2,2081) | 2:203:B:LEU:HD22 | 2:204:B:THR:H    | 15       | 0.17          |
| (2,2081) | 2:203:B:LEU:HD23 | 2:204:B:THR:H    | 15       | 0.17          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD11 | 17       | 0.17          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD12 | 17       | 0.17          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD13 | 17       | 0.17          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD21 | 17       | 0.17          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD22 | 17       | 0.17          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD23 | 17       | 0.17          |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD11 | 16       | 0.17          |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD12 | 16       | 0.17          |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD13 | 16       | 0.17          |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD21 | 16       | 0.17          |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD22 | 16       | 0.17          |
| (2,1934) | 1:74:A:PHE:H     | 2:214:B:LEU:HD23 | 16       | 0.17          |
| (2,1865) | 1:62:A:LEU:HB2   | 1:65:A:SER:HB2   | 7        | 0.17          |
| (2,1865) | 1:62:A:LEU:HB2   | 1:65:A:SER:HB3   | 7        | 0.17          |
| (2,1865) | 1:62:A:LEU:HB3   | 1:65:A:SER:HB2   | 7        | 0.17          |
| (2,1865) | 1:62:A:LEU:HB3   | 1:65:A:SER:HB3   | 7        | 0.17          |
| (2,1805) | 1:54:A:ILE:HG21  | 1:84:A:GLU:HB2   | 1        | 0.17          |
| (2,1805) | 1:54:A:ILE:HG21  | 1:84:A:GLU:HB3   | 1        | 0.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1805) | 1:54:A:ILE:HG22 | 1:84:A:GLU:HB2   | 1        | 0.17          |
| (2,1805) | 1:54:A:ILE:HG22 | 1:84:A:GLU:HB3   | 1        | 0.17          |
| (2,1805) | 1:54:A:ILE:HG23 | 1:84:A:GLU:HB2   | 1        | 0.17          |
| (2,1805) | 1:54:A:ILE:HG23 | 1:84:A:GLU:HB3   | 1        | 0.17          |
| (2,1805) | 1:54:A:ILE:HG21 | 1:84:A:GLU:HB2   | 19       | 0.17          |
| (2,1805) | 1:54:A:ILE:HG21 | 1:84:A:GLU:HB3   | 19       | 0.17          |
| (2,1805) | 1:54:A:ILE:HG22 | 1:84:A:GLU:HB2   | 19       | 0.17          |
| (2,1805) | 1:54:A:ILE:HG22 | 1:84:A:GLU:HB3   | 19       | 0.17          |
| (2,1805) | 1:54:A:ILE:HG23 | 1:84:A:GLU:HB2   | 19       | 0.17          |
| (2,1805) | 1:54:A:ILE:HG23 | 1:84:A:GLU:HB3   | 19       | 0.17          |
| (2,1728) | 1:48:A:LEU:HB2  | 2:205:B:TRP:HE1  | 6        | 0.17          |
| (2,1728) | 1:48:A:LEU:HB3  | 2:205:B:TRP:HE1  | 6        | 0.17          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD11  | 3        | 0.17          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD12  | 3        | 0.17          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD13  | 3        | 0.17          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD21  | 3        | 0.17          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD22  | 3        | 0.17          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD23  | 3        | 0.17          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD11  | 3        | 0.17          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD12  | 3        | 0.17          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD13  | 3        | 0.17          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD21  | 3        | 0.17          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD22  | 3        | 0.17          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD23  | 3        | 0.17          |
| (2,1602) | 1:34:A:ARG:HG3  | 2:213:B:PRO:HB2  | 2        | 0.17          |
| (2,1602) | 1:34:A:ARG:HG3  | 2:213:B:PRO:HB3  | 2        | 0.17          |
| (2,1500) | 1:20:A:GLU:HB2  | 1:21:A:GLU:H     | 9        | 0.17          |
| (2,1500) | 1:20:A:GLU:HB3  | 1:21:A:GLU:H     | 9        | 0.17          |
| (2,1451) | 1:71:A:GLU:HG3  | 2:218:B:LEU:H    | 15       | 0.17          |
| (2,1293) | 1:69:A:GLU:HG3  | 2:219:B:THR:HB   | 18       | 0.17          |
| (2,1267) | 2:205:B:TRP:HE3 | 2:220:B:ARG:HB3  | 19       | 0.17          |
| (2,1214) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD11 | 10       | 0.17          |
| (2,1214) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD12 | 10       | 0.17          |
| (2,1214) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD13 | 10       | 0.17          |
| (2,1208) | 2:215:B:LYS:HA  | 2:215:B:LYS:HD2  | 2        | 0.17          |
| (2,1160) | 2:204:B:THR:HA  | 2:205:B:TRP:HB3  | 20       | 0.17          |
| (2,1145) | 2:205:B:TRP:HE3 | 2:219:B:THR:HA   | 16       | 0.17          |
| (2,801)  | 1:74:A:PHE:H    | 2:214:B:LEU:HB2  | 14       | 0.17          |
| (2,799)  | 1:22:A:GLU:HB2  | 1:23:A:GLU:H     | 3        | 0.17          |
| (2,799)  | 1:22:A:GLU:HB2  | 1:23:A:GLU:H     | 17       | 0.17          |
| (2,568)  | 1:28:A:MET:HE1  | 1:82:A:LEU:H     | 18       | 0.17          |
| (2,568)  | 1:28:A:MET:HE2  | 1:82:A:LEU:H     | 18       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,568)  | 1:28:A:MET:HE3  | 1:82:A:LEU:H    | 18       | 0.17          |
| (2,304)  | 1:36:A:LEU:HA   | 1:39:A:ASP:HB3  | 1        | 0.17          |
| (2,256)  | 1:28:A:MET:HE1  | 1:33:A:LYS:HA   | 13       | 0.17          |
| (2,256)  | 1:28:A:MET:HE2  | 1:33:A:LYS:HA   | 13       | 0.17          |
| (2,256)  | 1:28:A:MET:HE3  | 1:33:A:LYS:HA   | 13       | 0.17          |
| (2,169)  | 1:74:A:PHE:HD1  | 1:77:A:LEU:HD21 | 18       | 0.17          |
| (2,169)  | 1:74:A:PHE:HD1  | 1:77:A:LEU:HD22 | 18       | 0.17          |
| (2,169)  | 1:74:A:PHE:HD1  | 1:77:A:LEU:HD23 | 18       | 0.17          |
| (2,169)  | 1:74:A:PHE:HD2  | 1:77:A:LEU:HD21 | 18       | 0.17          |
| (2,169)  | 1:74:A:PHE:HD2  | 1:77:A:LEU:HD22 | 18       | 0.17          |
| (2,169)  | 1:74:A:PHE:HD2  | 1:77:A:LEU:HD23 | 18       | 0.17          |
| (2,162)  | 1:52:A:VAL:HG11 | 2:205:B:TRP:HZ3 | 17       | 0.17          |
| (2,162)  | 1:52:A:VAL:HG12 | 2:205:B:TRP:HZ3 | 17       | 0.17          |
| (2,162)  | 1:52:A:VAL:HG13 | 2:205:B:TRP:HZ3 | 17       | 0.17          |
| (2,152)  | 1:34:A:ARG:HA   | 2:214:B:LEU:HG  | 1        | 0.17          |
| (2,9)    | 1:30:A:TYR:HE1  | 1:34:A:ARG:HG2  | 7        | 0.17          |
| (2,9)    | 1:30:A:TYR:HE2  | 1:34:A:ARG:HG2  | 7        | 0.17          |
| (1,22)   | 1:87:A:ARG:O    | 1:91:A:SER:H    | 20       | 0.17          |
| (1,21)   | 1:87:A:ARG:O    | 1:91:A:SER:N    | 20       | 0.17          |
| (1,10)   | 1:49:A:GLY:O    | 1:53:A:HIS:H    | 3        | 0.17          |
| (1,9)    | 1:49:A:GLY:O    | 1:53:A:HIS:N    | 19       | 0.17          |
| (2,2163) | 2:209:B:ARG:HG2 | 2:210:B:SER:HA  | 4        | 0.16          |
| (2,2163) | 2:209:B:ARG:HG3 | 2:210:B:SER:HA  | 4        | 0.16          |
| (2,2112) | 2:206:B:ARG:HD2 | 2:207:B:VAL:H   | 15       | 0.16          |
| (2,2112) | 2:206:B:ARG:HD3 | 2:207:B:VAL:H   | 15       | 0.16          |
| (2,2050) | 1:90:A:LYS:HA   | 1:90:A:LYS:HD2  | 1        | 0.16          |
| (2,2050) | 1:90:A:LYS:HA   | 1:90:A:LYS:HD3  | 1        | 0.16          |
| (2,1865) | 1:62:A:LEU:HB2  | 1:65:A:SER:HB2  | 8        | 0.16          |
| (2,1865) | 1:62:A:LEU:HB2  | 1:65:A:SER:HB3  | 8        | 0.16          |
| (2,1865) | 1:62:A:LEU:HB3  | 1:65:A:SER:HB2  | 8        | 0.16          |
| (2,1865) | 1:62:A:LEU:HB3  | 1:65:A:SER:HB3  | 8        | 0.16          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB2  | 13       | 0.16          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB3  | 13       | 0.16          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB2  | 13       | 0.16          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB3  | 13       | 0.16          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD11 | 8        | 0.16          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD12 | 8        | 0.16          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD13 | 8        | 0.16          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD21 | 8        | 0.16          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD22 | 8        | 0.16          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD23 | 8        | 0.16          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD11 | 8        | 0.16          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD12  | 8        | 0.16          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD13  | 8        | 0.16          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD21  | 8        | 0.16          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD22  | 8        | 0.16          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD23  | 8        | 0.16          |
| (2,1546) | 1:28:A:MET:HE1  | 1:33:A:LYS:HD2   | 12       | 0.16          |
| (2,1546) | 1:28:A:MET:HE1  | 1:33:A:LYS:HD3   | 12       | 0.16          |
| (2,1546) | 1:28:A:MET:HE2  | 1:33:A:LYS:HD2   | 12       | 0.16          |
| (2,1546) | 1:28:A:MET:HE2  | 1:33:A:LYS:HD3   | 12       | 0.16          |
| (2,1546) | 1:28:A:MET:HE3  | 1:33:A:LYS:HD2   | 12       | 0.16          |
| (2,1546) | 1:28:A:MET:HE3  | 1:33:A:LYS:HD3   | 12       | 0.16          |
| (2,1500) | 1:20:A:GLU:HB2  | 1:21:A:GLU:H     | 5        | 0.16          |
| (2,1500) | 1:20:A:GLU:HB3  | 1:21:A:GLU:H     | 5        | 0.16          |
| (2,1418) | 2:214:B:LEU:H   | 2:215:B:LYS:HB2  | 7        | 0.16          |
| (2,1358) | 2:205:B:TRP:HD1 | 2:206:B:ARG:H    | 14       | 0.16          |
| (2,1356) | 2:205:B:TRP:HE3 | 2:220:B:ARG:H    | 7        | 0.16          |
| (2,1335) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD11 | 12       | 0.16          |
| (2,1335) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD12 | 12       | 0.16          |
| (2,1335) | 2:213:B:PRO:HG3 | 2:214:B:LEU:HD13 | 12       | 0.16          |
| (2,1322) | 2:221:B:GLU:HB3 | 2:222:B:ALA:HA   | 11       | 0.16          |
| (2,1321) | 2:221:B:GLU:HB2 | 2:222:B:ALA:H    | 17       | 0.16          |
| (2,1293) | 1:69:A:GLU:HG3  | 2:219:B:THR:HB   | 12       | 0.16          |
| (2,1265) | 2:204:B:THR:HB  | 2:205:B:TRP:HB3  | 4        | 0.16          |
| (2,1247) | 1:30:A:TYR:HA   | 2:214:B:LEU:HD11 | 3        | 0.16          |
| (2,1247) | 1:30:A:TYR:HA   | 2:214:B:LEU:HD12 | 3        | 0.16          |
| (2,1247) | 1:30:A:TYR:HA   | 2:214:B:LEU:HD13 | 3        | 0.16          |
| (2,1225) | 1:73:A:ASP:HB3  | 2:215:B:LYS:HA   | 15       | 0.16          |
| (2,1208) | 2:215:B:LYS:HA  | 2:215:B:LYS:HD2  | 12       | 0.16          |
| (2,1187) | 2:217:B:ARG:HG2 | 2:218:B:LEU:H    | 16       | 0.16          |
| (2,1161) | 1:68:A:ASP:HB2  | 2:220:B:ARG:HB2  | 3        | 0.16          |
| (2,1160) | 2:204:B:THR:HA  | 2:205:B:TRP:HB3  | 8        | 0.16          |
| (2,752)  | 1:75:A:GLU:H    | 2:214:B:LEU:HG   | 19       | 0.16          |
| (2,747)  | 1:33:A:LYS:H    | 1:33:A:LYS:HD3   | 10       | 0.16          |
| (2,670)  | 1:28:A:MET:HB2  | 1:33:A:LYS:HE3   | 4        | 0.16          |
| (2,553)  | 1:27:A:PRO:HA   | 1:79:A:PRO:HB3   | 13       | 0.16          |
| (2,432)  | 1:53:A:HIS:HA   | 1:56:A:GLN:HB3   | 3        | 0.16          |
| (2,169)  | 1:74:A:PHE:HD1  | 1:77:A:LEU:HD21  | 12       | 0.16          |
| (2,169)  | 1:74:A:PHE:HD1  | 1:77:A:LEU:HD22  | 12       | 0.16          |
| (2,169)  | 1:74:A:PHE:HD1  | 1:77:A:LEU:HD23  | 12       | 0.16          |
| (2,169)  | 1:74:A:PHE:HD2  | 1:77:A:LEU:HD21  | 12       | 0.16          |
| (2,169)  | 1:74:A:PHE:HD2  | 1:77:A:LEU:HD22  | 12       | 0.16          |
| (2,169)  | 1:74:A:PHE:HD2  | 1:77:A:LEU:HD23  | 12       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,152)  | 1:34:A:ARG:HA    | 2:214:B:LEU:HG   | 6        | 0.16          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 14       | 0.16          |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H     | 12       | 0.16          |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H     | 18       | 0.16          |
| (1,9)    | 1:49:A:GLY:O     | 1:53:A:HIS:N     | 8        | 0.16          |
| (2,2199) | 2:214:B:LEU:HD11 | 2:215:B:LYS:H    | 7        | 0.15          |
| (2,2199) | 2:214:B:LEU:HD12 | 2:215:B:LYS:H    | 7        | 0.15          |
| (2,2199) | 2:214:B:LEU:HD13 | 2:215:B:LYS:H    | 7        | 0.15          |
| (2,2199) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H    | 7        | 0.15          |
| (2,2199) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H    | 7        | 0.15          |
| (2,2199) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H    | 7        | 0.15          |
| (2,2108) | 2:206:B:ARG:HG2  | 2:207:B:VAL:H    | 8        | 0.15          |
| (2,2108) | 2:206:B:ARG:HG3  | 2:207:B:VAL:H    | 8        | 0.15          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD11 | 15       | 0.15          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD12 | 15       | 0.15          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD13 | 15       | 0.15          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD21 | 15       | 0.15          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD22 | 15       | 0.15          |
| (2,2101) | 2:206:B:ARG:H    | 2:218:B:LEU:HD23 | 15       | 0.15          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD11 | 18       | 0.15          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD12 | 18       | 0.15          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD13 | 18       | 0.15          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD21 | 18       | 0.15          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD22 | 18       | 0.15          |
| (2,2097) | 2:205:B:TRP:HH2  | 2:218:B:LEU:HD23 | 18       | 0.15          |
| (2,2050) | 1:90:A:LYS:HA    | 1:90:A:LYS:HD2   | 13       | 0.15          |
| (2,2050) | 1:90:A:LYS:HA    | 1:90:A:LYS:HD3   | 13       | 0.15          |
| (2,2015) | 1:86:A:GLU:HA    | 1:89:A:VAL:HG11  | 4        | 0.15          |
| (2,2015) | 1:86:A:GLU:HA    | 1:89:A:VAL:HG12  | 4        | 0.15          |
| (2,2015) | 1:86:A:GLU:HA    | 1:89:A:VAL:HG13  | 4        | 0.15          |
| (2,2015) | 1:86:A:GLU:HA    | 1:89:A:VAL:HG21  | 4        | 0.15          |
| (2,2015) | 1:86:A:GLU:HA    | 1:89:A:VAL:HG22  | 4        | 0.15          |
| (2,2015) | 1:86:A:GLU:HA    | 1:89:A:VAL:HG23  | 4        | 0.15          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD11 | 7        | 0.15          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD12 | 7        | 0.15          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD13 | 7        | 0.15          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD21 | 7        | 0.15          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD22 | 7        | 0.15          |
| (2,1955) | 1:75:A:GLU:HG3   | 2:214:B:LEU:HD23 | 7        | 0.15          |
| (2,1737) | 1:48:A:LEU:HD11  | 2:205:B:TRP:HZ2  | 14       | 0.15          |
| (2,1737) | 1:48:A:LEU:HD12  | 2:205:B:TRP:HZ2  | 14       | 0.15          |
| (2,1737) | 1:48:A:LEU:HD13  | 2:205:B:TRP:HZ2  | 14       | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1737) | 1:48:A:LEU:HD21 | 2:205:B:TRP:HZ2  | 14       | 0.15          |
| (2,1737) | 1:48:A:LEU:HD22 | 2:205:B:TRP:HZ2  | 14       | 0.15          |
| (2,1737) | 1:48:A:LEU:HD23 | 2:205:B:TRP:HZ2  | 14       | 0.15          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB2   | 2        | 0.15          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB3   | 2        | 0.15          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB2   | 2        | 0.15          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB3   | 2        | 0.15          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB2   | 8        | 0.15          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB3   | 8        | 0.15          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB2   | 8        | 0.15          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB3   | 8        | 0.15          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD11  | 18       | 0.15          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD12  | 18       | 0.15          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD13  | 18       | 0.15          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD21  | 18       | 0.15          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD22  | 18       | 0.15          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD23  | 18       | 0.15          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD11  | 18       | 0.15          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD12  | 18       | 0.15          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD13  | 18       | 0.15          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD21  | 18       | 0.15          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD22  | 18       | 0.15          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD23  | 18       | 0.15          |
| (2,1612) | 1:35:A:GLN:HA   | 1:39:A:ASP:HB2   | 4        | 0.15          |
| (2,1612) | 1:35:A:GLN:HA   | 1:39:A:ASP:HB3   | 4        | 0.15          |
| (2,1599) | 1:34:A:ARG:HB3  | 1:38:A:LEU:HD11  | 12       | 0.15          |
| (2,1599) | 1:34:A:ARG:HB3  | 1:38:A:LEU:HD12  | 12       | 0.15          |
| (2,1599) | 1:34:A:ARG:HB3  | 1:38:A:LEU:HD13  | 12       | 0.15          |
| (2,1599) | 1:34:A:ARG:HB3  | 1:38:A:LEU:HD21  | 12       | 0.15          |
| (2,1599) | 1:34:A:ARG:HB3  | 1:38:A:LEU:HD22  | 12       | 0.15          |
| (2,1599) | 1:34:A:ARG:HB3  | 1:38:A:LEU:HD23  | 12       | 0.15          |
| (2,1500) | 1:20:A:GLU:HB2  | 1:21:A:GLU:H     | 18       | 0.15          |
| (2,1500) | 1:20:A:GLU:HB3  | 1:21:A:GLU:H     | 18       | 0.15          |
| (2,1392) | 2:209:B:ARG:HD3 | 2:210:B:SER:H    | 3        | 0.15          |
| (2,1392) | 2:209:B:ARG:HD3 | 2:210:B:SER:H    | 20       | 0.15          |
| (2,1391) | 2:209:B:ARG:HD2 | 2:210:B:SER:H    | 3        | 0.15          |
| (2,1386) | 2:204:B:THR:HB  | 2:205:B:TRP:H    | 6        | 0.15          |
| (2,1300) | 1:73:A:ASP:HA   | 2:216:B:ILE:HG12 | 13       | 0.15          |
| (2,1293) | 1:69:A:GLU:HG3  | 2:219:B:THR:HB   | 20       | 0.15          |
| (2,1287) | 1:48:A:LEU:HA   | 2:218:B:LEU:HG   | 11       | 0.15          |
| (2,1280) | 1:72:A:ILE:HG21 | 2:216:B:ILE:HB   | 13       | 0.15          |
| (2,1280) | 1:72:A:ILE:HG22 | 2:216:B:ILE:HB   | 13       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1280) | 1:72:A:ILE:HG23  | 2:216:B:ILE:HB   | 13       | 0.15          |
| (2,1280) | 1:72:A:ILE:HG21  | 2:216:B:ILE:HB   | 15       | 0.15          |
| (2,1280) | 1:72:A:ILE:HG22  | 2:216:B:ILE:HB   | 15       | 0.15          |
| (2,1280) | 1:72:A:ILE:HG23  | 2:216:B:ILE:HB   | 15       | 0.15          |
| (2,1237) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB2  | 15       | 0.15          |
| (2,1214) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD11 | 7        | 0.15          |
| (2,1214) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD12 | 7        | 0.15          |
| (2,1214) | 1:75:A:GLU:HB3   | 2:214:B:LEU:HD13 | 7        | 0.15          |
| (2,1187) | 2:217:B:ARG:HG2  | 2:218:B:LEU:H    | 17       | 0.15          |
| (2,1148) | 2:217:B:ARG:HD2  | 2:219:B:THR:HG21 | 7        | 0.15          |
| (2,1148) | 2:217:B:ARG:HD2  | 2:219:B:THR:HG22 | 7        | 0.15          |
| (2,1148) | 2:217:B:ARG:HD2  | 2:219:B:THR:HG23 | 7        | 0.15          |
| (2,619)  | 1:72:A:ILE:HB    | 2:216:B:ILE:HB   | 19       | 0.15          |
| (2,310)  | 1:37:A:SER:HA    | 1:40:A:ILE:HD11  | 15       | 0.15          |
| (2,310)  | 1:37:A:SER:HA    | 1:40:A:ILE:HD12  | 15       | 0.15          |
| (2,310)  | 1:37:A:SER:HA    | 1:40:A:ILE:HD13  | 15       | 0.15          |
| (2,198)  | 1:39:A:ASP:HA    | 1:93:A:LEU:HD11  | 15       | 0.15          |
| (2,198)  | 1:39:A:ASP:HA    | 1:93:A:LEU:HD12  | 15       | 0.15          |
| (2,198)  | 1:39:A:ASP:HA    | 1:93:A:LEU:HD13  | 15       | 0.15          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD21  | 9        | 0.15          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD22  | 9        | 0.15          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD23  | 9        | 0.15          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD21  | 9        | 0.15          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD22  | 9        | 0.15          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD23  | 9        | 0.15          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD21  | 14       | 0.15          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD22  | 14       | 0.15          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD23  | 14       | 0.15          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD21  | 14       | 0.15          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD22  | 14       | 0.15          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD23  | 14       | 0.15          |
| (2,30)   | 1:30:A:TYR:HE1   | 2:214:B:LEU:HG   | 7        | 0.15          |
| (2,30)   | 1:30:A:TYR:HE2   | 2:214:B:LEU:HG   | 7        | 0.15          |
| (2,12)   | 2:204:B:THR:HB   | 2:205:B:TRP:HD1  | 7        | 0.15          |
| (1,14)   | 1:51:A:VAL:O     | 1:55:A:ILE:H     | 3        | 0.15          |
| (1,11)   | 1:50:A:ARG:O     | 1:54:A:ILE:N     | 2        | 0.15          |
| (1,3)    | 1:34:A:ARG:O     | 1:38:A:LEU:N     | 14       | 0.15          |
| (2,2199) | 2:214:B:LEU:HD11 | 2:215:B:LYS:H    | 10       | 0.14          |
| (2,2199) | 2:214:B:LEU:HD12 | 2:215:B:LYS:H    | 10       | 0.14          |
| (2,2199) | 2:214:B:LEU:HD13 | 2:215:B:LYS:H    | 10       | 0.14          |
| (2,2199) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H    | 10       | 0.14          |
| (2,2199) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H    | 10       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2199) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H    | 10       | 0.14          |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD11 | 18       | 0.14          |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD12 | 18       | 0.14          |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD13 | 18       | 0.14          |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD21 | 18       | 0.14          |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD22 | 18       | 0.14          |
| (2,2196) | 2:214:B:LEU:H    | 2:214:B:LEU:HD23 | 18       | 0.14          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD11 | 5        | 0.14          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD12 | 5        | 0.14          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD13 | 5        | 0.14          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD21 | 5        | 0.14          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD22 | 5        | 0.14          |
| (2,2192) | 2:213:B:PRO:HG2  | 2:214:B:LEU:HD23 | 5        | 0.14          |
| (2,2175) | 2:211:B:GLN:HG2  | 2:212:B:ASN:H    | 17       | 0.14          |
| (2,2175) | 2:211:B:GLN:HG3  | 2:212:B:ASN:H    | 17       | 0.14          |
| (2,2171) | 2:210:B:SER:HB2  | 2:215:B:LYS:HB2  | 6        | 0.14          |
| (2,2171) | 2:210:B:SER:HB3  | 2:215:B:LYS:HB2  | 6        | 0.14          |
| (2,2148) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HB3  | 3        | 0.14          |
| (2,2148) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HB3  | 3        | 0.14          |
| (2,2050) | 1:90:A:LYS:HA    | 1:90:A:LYS:HD2   | 15       | 0.14          |
| (2,2050) | 1:90:A:LYS:HA    | 1:90:A:LYS:HD3   | 15       | 0.14          |
| (2,2032) | 1:87:A:ARG:HD2   | 1:88:A:TYR:HD1   | 15       | 0.14          |
| (2,2032) | 1:87:A:ARG:HD2   | 1:88:A:TYR:HD2   | 15       | 0.14          |
| (2,2032) | 1:87:A:ARG:HD3   | 1:88:A:TYR:HD1   | 15       | 0.14          |
| (2,2032) | 1:87:A:ARG:HD3   | 1:88:A:TYR:HD2   | 15       | 0.14          |
| (2,1965) | 1:77:A:LEU:HD11  | 1:78:A:LYS:HB2   | 9        | 0.14          |
| (2,1965) | 1:77:A:LEU:HD12  | 1:78:A:LYS:HB2   | 9        | 0.14          |
| (2,1965) | 1:77:A:LEU:HD13  | 1:78:A:LYS:HB2   | 9        | 0.14          |
| (2,1965) | 1:77:A:LEU:HD21  | 1:78:A:LYS:HB2   | 9        | 0.14          |
| (2,1965) | 1:77:A:LEU:HD22  | 1:78:A:LYS:HB2   | 9        | 0.14          |
| (2,1965) | 1:77:A:LEU:HD23  | 1:78:A:LYS:HB2   | 9        | 0.14          |
| (2,1736) | 1:48:A:LEU:HD11  | 2:205:B:TRP:H    | 3        | 0.14          |
| (2,1736) | 1:48:A:LEU:HD12  | 2:205:B:TRP:H    | 3        | 0.14          |
| (2,1736) | 1:48:A:LEU:HD13  | 2:205:B:TRP:H    | 3        | 0.14          |
| (2,1736) | 1:48:A:LEU:HD21  | 2:205:B:TRP:H    | 3        | 0.14          |
| (2,1736) | 1:48:A:LEU:HD22  | 2:205:B:TRP:H    | 3        | 0.14          |
| (2,1736) | 1:48:A:LEU:HD23  | 2:205:B:TRP:H    | 3        | 0.14          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD11 | 6        | 0.14          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD12 | 6        | 0.14          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD13 | 6        | 0.14          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD21 | 6        | 0.14          |
| (2,1653) | 1:37:A:SER:H     | 2:214:B:LEU:HD22 | 6        | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1653) | 1:37:A:SER:H    | 2:214:B:LEU:HD23 | 6        | 0.14          |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD11 | 6        | 0.14          |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD12 | 6        | 0.14          |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD13 | 6        | 0.14          |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD21 | 6        | 0.14          |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD22 | 6        | 0.14          |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD23 | 6        | 0.14          |
| (2,1612) | 1:35:A:GLN:HA   | 1:39:A:ASP:HB2   | 14       | 0.14          |
| (2,1612) | 1:35:A:GLN:HA   | 1:39:A:ASP:HB3   | 14       | 0.14          |
| (2,1546) | 1:28:A:MET:HE1  | 1:33:A:LYS:HD2   | 3        | 0.14          |
| (2,1546) | 1:28:A:MET:HE1  | 1:33:A:LYS:HD3   | 3        | 0.14          |
| (2,1546) | 1:28:A:MET:HE2  | 1:33:A:LYS:HD2   | 3        | 0.14          |
| (2,1546) | 1:28:A:MET:HE2  | 1:33:A:LYS:HD3   | 3        | 0.14          |
| (2,1546) | 1:28:A:MET:HE3  | 1:33:A:LYS:HD2   | 3        | 0.14          |
| (2,1546) | 1:28:A:MET:HE3  | 1:33:A:LYS:HD3   | 3        | 0.14          |
| (2,1545) | 1:28:A:MET:HE1  | 1:33:A:LYS:HG2   | 4        | 0.14          |
| (2,1545) | 1:28:A:MET:HE1  | 1:33:A:LYS:HG3   | 4        | 0.14          |
| (2,1545) | 1:28:A:MET:HE2  | 1:33:A:LYS:HG2   | 4        | 0.14          |
| (2,1545) | 1:28:A:MET:HE2  | 1:33:A:LYS:HG3   | 4        | 0.14          |
| (2,1545) | 1:28:A:MET:HE3  | 1:33:A:LYS:HG2   | 4        | 0.14          |
| (2,1545) | 1:28:A:MET:HE3  | 1:33:A:LYS:HG3   | 4        | 0.14          |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD11  | 6        | 0.14          |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD12  | 6        | 0.14          |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD13  | 6        | 0.14          |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD21  | 6        | 0.14          |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD22  | 6        | 0.14          |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD23  | 6        | 0.14          |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG2   | 9        | 0.14          |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG3   | 9        | 0.14          |
| (2,1526) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HG2   | 9        | 0.14          |
| (2,1526) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HG3   | 9        | 0.14          |
| (2,1526) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HG2   | 9        | 0.14          |
| (2,1526) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HG3   | 9        | 0.14          |
| (2,1526) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HG2   | 9        | 0.14          |
| (2,1526) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HG3   | 9        | 0.14          |
| (2,1526) | 1:26:A:LEU:HD22 | 1:27:A:PRO:HG2   | 9        | 0.14          |
| (2,1526) | 1:26:A:LEU:HD22 | 1:27:A:PRO:HG3   | 9        | 0.14          |
| (2,1526) | 1:26:A:LEU:HD23 | 1:27:A:PRO:HG2   | 9        | 0.14          |
| (2,1526) | 1:26:A:LEU:HD23 | 1:27:A:PRO:HG3   | 9        | 0.14          |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG2   | 10       | 0.14          |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG3   | 10       | 0.14          |
| (2,1526) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HG2   | 10       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1526) | 1:26:A:LEU:HD12  | 1:27:A:PRO:HG3   | 10       | 0.14          |
| (2,1526) | 1:26:A:LEU:HD13  | 1:27:A:PRO:HG2   | 10       | 0.14          |
| (2,1526) | 1:26:A:LEU:HD13  | 1:27:A:PRO:HG3   | 10       | 0.14          |
| (2,1526) | 1:26:A:LEU:HD21  | 1:27:A:PRO:HG2   | 10       | 0.14          |
| (2,1526) | 1:26:A:LEU:HD21  | 1:27:A:PRO:HG3   | 10       | 0.14          |
| (2,1526) | 1:26:A:LEU:HD22  | 1:27:A:PRO:HG2   | 10       | 0.14          |
| (2,1526) | 1:26:A:LEU:HD22  | 1:27:A:PRO:HG3   | 10       | 0.14          |
| (2,1526) | 1:26:A:LEU:HD23  | 1:27:A:PRO:HG2   | 10       | 0.14          |
| (2,1526) | 1:26:A:LEU:HD23  | 1:27:A:PRO:HG3   | 10       | 0.14          |
| (2,1503) | 1:22:A:GLU:HB2   | 1:23:A:GLU:H     | 20       | 0.14          |
| (2,1503) | 1:22:A:GLU:HB3   | 1:23:A:GLU:H     | 20       | 0.14          |
| (2,1485) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HG3  | 2        | 0.14          |
| (2,1428) | 2:208:B:GLN:H    | 2:219:B:THR:HG21 | 19       | 0.14          |
| (2,1428) | 2:208:B:GLN:H    | 2:219:B:THR:HG22 | 19       | 0.14          |
| (2,1428) | 2:208:B:GLN:H    | 2:219:B:THR:HG23 | 19       | 0.14          |
| (2,1403) | 2:221:B:GLU:HB3  | 2:222:B:ALA:H    | 7        | 0.14          |
| (2,1367) | 1:73:A:ASP:HA    | 2:215:B:LYS:H    | 1        | 0.14          |
| (2,1331) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD21 | 14       | 0.14          |
| (2,1331) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD22 | 14       | 0.14          |
| (2,1331) | 2:207:B:VAL:HB   | 2:218:B:LEU:HD23 | 14       | 0.14          |
| (2,1321) | 2:221:B:GLU:HB2  | 2:222:B:ALA:H    | 5        | 0.14          |
| (2,1321) | 2:221:B:GLU:HB2  | 2:222:B:ALA:H    | 8        | 0.14          |
| (2,1321) | 2:221:B:GLU:HB2  | 2:222:B:ALA:H    | 11       | 0.14          |
| (2,1287) | 1:48:A:LEU:HA    | 2:218:B:LEU:HG   | 18       | 0.14          |
| (2,1176) | 2:210:B:SER:HB2  | 2:215:B:LYS:HB3  | 10       | 0.14          |
| (2,679)  | 1:34:A:ARG:H     | 2:214:B:LEU:HD11 | 14       | 0.14          |
| (2,679)  | 1:34:A:ARG:H     | 2:214:B:LEU:HD12 | 14       | 0.14          |
| (2,679)  | 1:34:A:ARG:H     | 2:214:B:LEU:HD13 | 14       | 0.14          |
| (2,633)  | 1:71:A:GLU:HG3   | 2:217:B:ARG:HG2  | 1        | 0.14          |
| (2,553)  | 1:27:A:PRO:HA    | 1:79:A:PRO:HB3   | 2        | 0.14          |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD11 | 2        | 0.14          |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD12 | 2        | 0.14          |
| (2,536)  | 1:74:A:PHE:HB2   | 2:214:B:LEU:HD13 | 2        | 0.14          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD21  | 2        | 0.14          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD22  | 2        | 0.14          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD23  | 2        | 0.14          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD21  | 2        | 0.14          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD22  | 2        | 0.14          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD23  | 2        | 0.14          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD21  | 6        | 0.14          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD22  | 6        | 0.14          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD23  | 6        | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD21 | 6        | 0.14          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD22 | 6        | 0.14          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD23 | 6        | 0.14          |
| (2,30)   | 1:30:A:TYR:HE1   | 2:214:B:LEU:HG  | 4        | 0.14          |
| (2,30)   | 1:30:A:TYR:HE2   | 2:214:B:LEU:HG  | 4        | 0.14          |
| (1,22)   | 1:87:A:ARG:O     | 1:91:A:SER:H    | 10       | 0.14          |
| (1,22)   | 1:87:A:ARG:O     | 1:91:A:SER:H    | 18       | 0.14          |
| (1,21)   | 1:87:A:ARG:O     | 1:91:A:SER:N    | 9        | 0.14          |
| (1,10)   | 1:49:A:GLY:O     | 1:53:A:HIS:H    | 5        | 0.14          |
| (2,2148) | 2:208:B:GLN:HG2  | 2:217:B:ARG:HB3 | 18       | 0.13          |
| (2,2148) | 2:208:B:GLN:HG3  | 2:217:B:ARG:HB3 | 18       | 0.13          |
| (2,2138) | 2:208:B:GLN:HB2  | 2:217:B:ARG:HB3 | 6        | 0.13          |
| (2,2138) | 2:208:B:GLN:HB3  | 2:217:B:ARG:HB3 | 6        | 0.13          |
| (2,2113) | 2:206:B:ARG:HD2  | 2:221:B:GLU:HG2 | 11       | 0.13          |
| (2,2113) | 2:206:B:ARG:HD2  | 2:221:B:GLU:HG3 | 11       | 0.13          |
| (2,2113) | 2:206:B:ARG:HD3  | 2:221:B:GLU:HG2 | 11       | 0.13          |
| (2,2113) | 2:206:B:ARG:HD3  | 2:221:B:GLU:HG3 | 11       | 0.13          |
| (2,2095) | 2:205:B:TRP:HE3  | 2:220:B:ARG:HD2 | 16       | 0.13          |
| (2,2095) | 2:205:B:TRP:HE3  | 2:220:B:ARG:HD3 | 16       | 0.13          |
| (2,2081) | 2:203:B:LEU:HD11 | 2:204:B:THR:H   | 6        | 0.13          |
| (2,2081) | 2:203:B:LEU:HD12 | 2:204:B:THR:H   | 6        | 0.13          |
| (2,2081) | 2:203:B:LEU:HD13 | 2:204:B:THR:H   | 6        | 0.13          |
| (2,2081) | 2:203:B:LEU:HD21 | 2:204:B:THR:H   | 6        | 0.13          |
| (2,2081) | 2:203:B:LEU:HD22 | 2:204:B:THR:H   | 6        | 0.13          |
| (2,2081) | 2:203:B:LEU:HD23 | 2:204:B:THR:H   | 6        | 0.13          |
| (2,2029) | 1:87:A:ARG:HG2   | 1:88:A:TYR:HA   | 3        | 0.13          |
| (2,2029) | 1:87:A:ARG:HG3   | 1:88:A:TYR:HA   | 3        | 0.13          |
| (2,1930) | 1:73:A:ASP:HB2   | 2:215:B:LYS:HG2 | 9        | 0.13          |
| (2,1930) | 1:73:A:ASP:HB3   | 2:215:B:LYS:HG2 | 9        | 0.13          |
| (2,1924) | 1:73:A:ASP:HB2   | 1:75:A:GLU:HG2  | 9        | 0.13          |
| (2,1924) | 1:73:A:ASP:HB3   | 1:75:A:GLU:HG2  | 9        | 0.13          |
| (2,1915) | 1:71:A:GLU:HG2   | 2:217:B:ARG:HD2 | 8        | 0.13          |
| (2,1915) | 1:71:A:GLU:HG2   | 2:217:B:ARG:HD3 | 8        | 0.13          |
| (2,1805) | 1:54:A:ILE:HG21  | 1:84:A:GLU:HB2  | 8        | 0.13          |
| (2,1805) | 1:54:A:ILE:HG21  | 1:84:A:GLU:HB3  | 8        | 0.13          |
| (2,1805) | 1:54:A:ILE:HG22  | 1:84:A:GLU:HB2  | 8        | 0.13          |
| (2,1805) | 1:54:A:ILE:HG22  | 1:84:A:GLU:HB3  | 8        | 0.13          |
| (2,1805) | 1:54:A:ILE:HG23  | 1:84:A:GLU:HB2  | 8        | 0.13          |
| (2,1805) | 1:54:A:ILE:HG23  | 1:84:A:GLU:HB3  | 8        | 0.13          |
| (2,1728) | 1:48:A:LEU:HB2   | 2:205:B:TRP:HE1 | 2        | 0.13          |
| (2,1728) | 1:48:A:LEU:HB3   | 2:205:B:TRP:HE1 | 2        | 0.13          |
| (2,1631) | 1:36:A:LEU:HB2   | 1:40:A:ILE:HD11 | 3        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1631) | 1:36:A:LEU:HB2  | 1:40:A:ILE:HD12 | 3        | 0.13          |
| (2,1631) | 1:36:A:LEU:HB2  | 1:40:A:ILE:HD13 | 3        | 0.13          |
| (2,1631) | 1:36:A:LEU:HB3  | 1:40:A:ILE:HD11 | 3        | 0.13          |
| (2,1631) | 1:36:A:LEU:HB3  | 1:40:A:ILE:HD12 | 3        | 0.13          |
| (2,1631) | 1:36:A:LEU:HB3  | 1:40:A:ILE:HD13 | 3        | 0.13          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB2  | 1        | 0.13          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB3  | 1        | 0.13          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB2  | 1        | 0.13          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB3  | 1        | 0.13          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD11 | 9        | 0.13          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD12 | 9        | 0.13          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD13 | 9        | 0.13          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD21 | 9        | 0.13          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD22 | 9        | 0.13          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD23 | 9        | 0.13          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD11 | 9        | 0.13          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD12 | 9        | 0.13          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD13 | 9        | 0.13          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD21 | 9        | 0.13          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD22 | 9        | 0.13          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD23 | 9        | 0.13          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD11 | 14       | 0.13          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD12 | 14       | 0.13          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD13 | 14       | 0.13          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD21 | 14       | 0.13          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD22 | 14       | 0.13          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD23 | 14       | 0.13          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD11 | 14       | 0.13          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD12 | 14       | 0.13          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD13 | 14       | 0.13          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD21 | 14       | 0.13          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD22 | 14       | 0.13          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD23 | 14       | 0.13          |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG2  | 4        | 0.13          |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG3  | 4        | 0.13          |
| (2,1526) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HG2  | 4        | 0.13          |
| (2,1526) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HG3  | 4        | 0.13          |
| (2,1526) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HG2  | 4        | 0.13          |
| (2,1526) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HG3  | 4        | 0.13          |
| (2,1526) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HG2  | 4        | 0.13          |
| (2,1526) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HG3  | 4        | 0.13          |
| (2,1526) | 1:26:A:LEU:HD22 | 1:27:A:PRO:HG2  | 4        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1526) | 1:26:A:LEU:HD22  | 1:27:A:PRO:HG3   | 4        | 0.13          |
| (2,1526) | 1:26:A:LEU:HD23  | 1:27:A:PRO:HG2   | 4        | 0.13          |
| (2,1526) | 1:26:A:LEU:HD23  | 1:27:A:PRO:HG3   | 4        | 0.13          |
| (2,1487) | 2:212:B:ASN:HD21 | 2:215:B:LYS:HB2  | 5        | 0.13          |
| (2,1463) | 2:211:B:GLN:HG3  | 2:212:B:ASN:H    | 17       | 0.13          |
| (2,1437) | 2:214:B:LEU:H    | 2:214:B:LEU:HD21 | 18       | 0.13          |
| (2,1437) | 2:214:B:LEU:H    | 2:214:B:LEU:HD22 | 18       | 0.13          |
| (2,1437) | 2:214:B:LEU:H    | 2:214:B:LEU:HD23 | 18       | 0.13          |
| (2,1419) | 2:208:B:GLN:H    | 2:218:B:LEU:HG   | 8        | 0.13          |
| (2,1386) | 2:204:B:THR:HB   | 2:205:B:TRP:H    | 19       | 0.13          |
| (2,1253) | 2:214:B:LEU:HG   | 2:215:B:LYS:H    | 11       | 0.13          |
| (2,1206) | 1:73:A:ASP:HA    | 2:215:B:LYS:HG3  | 7        | 0.13          |
| (2,1187) | 2:217:B:ARG:HG2  | 2:218:B:LEU:H    | 11       | 0.13          |
| (2,784)  | 1:35:A:GLN:HE22  | 1:38:A:LEU:HB2   | 14       | 0.13          |
| (2,743)  | 1:70:A:ILE:H     | 2:218:B:LEU:HB2  | 5        | 0.13          |
| (2,553)  | 1:27:A:PRO:HA    | 1:79:A:PRO:HB3   | 16       | 0.13          |
| (2,432)  | 1:53:A:HIS:HA    | 1:56:A:GLN:HB3   | 2        | 0.13          |
| (2,310)  | 1:37:A:SER:HA    | 1:40:A:ILE:HD11  | 7        | 0.13          |
| (2,310)  | 1:37:A:SER:HA    | 1:40:A:ILE:HD12  | 7        | 0.13          |
| (2,310)  | 1:37:A:SER:HA    | 1:40:A:ILE:HD13  | 7        | 0.13          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD21  | 1        | 0.13          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD22  | 1        | 0.13          |
| (2,169)  | 1:74:A:PHE:HD1   | 1:77:A:LEU:HD23  | 1        | 0.13          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD21  | 1        | 0.13          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD22  | 1        | 0.13          |
| (2,169)  | 1:74:A:PHE:HD2   | 1:77:A:LEU:HD23  | 1        | 0.13          |
| (2,65)   | 1:36:A:LEU:HG    | 1:40:A:ILE:HD11  | 13       | 0.13          |
| (2,65)   | 1:36:A:LEU:HG    | 1:40:A:ILE:HD12  | 13       | 0.13          |
| (2,65)   | 1:36:A:LEU:HG    | 1:40:A:ILE:HD13  | 13       | 0.13          |
| (2,35)   | 1:54:A:ILE:HD11  | 1:55:A:ILE:HG12  | 12       | 0.13          |
| (2,35)   | 1:54:A:ILE:HD12  | 1:55:A:ILE:HG12  | 12       | 0.13          |
| (2,35)   | 1:54:A:ILE:HD13  | 1:55:A:ILE:HG12  | 12       | 0.13          |
| (1,22)   | 1:87:A:ARG:O     | 1:91:A:SER:H     | 9        | 0.13          |
| (1,18)   | 1:53:A:HIS:O     | 1:57:A:SER:H     | 2        | 0.13          |
| (1,3)    | 1:34:A:ARG:O     | 1:38:A:LEU:N     | 7        | 0.13          |
| (1,3)    | 1:34:A:ARG:O     | 1:38:A:LEU:N     | 9        | 0.13          |
| (2,2185) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HG3  | 17       | 0.12          |
| (2,2185) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HG3  | 17       | 0.12          |
| (2,2184) | 2:212:B:ASN:HB2  | 2:215:B:LYS:HB3  | 5        | 0.12          |
| (2,2184) | 2:212:B:ASN:HB3  | 2:215:B:LYS:HB3  | 5        | 0.12          |
| (2,2127) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HG   | 11       | 0.12          |
| (2,2127) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HG   | 11       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,2127) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HG   | 11       | 0.12          |
| (2,2127) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HG   | 11       | 0.12          |
| (2,2127) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HG   | 11       | 0.12          |
| (2,2127) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HG   | 11       | 0.12          |
| (2,2122) | 2:207:B:VAL:HG11 | 2:217:B:ARG:H    | 19       | 0.12          |
| (2,2122) | 2:207:B:VAL:HG12 | 2:217:B:ARG:H    | 19       | 0.12          |
| (2,2122) | 2:207:B:VAL:HG13 | 2:217:B:ARG:H    | 19       | 0.12          |
| (2,2122) | 2:207:B:VAL:HG21 | 2:217:B:ARG:H    | 19       | 0.12          |
| (2,2122) | 2:207:B:VAL:HG22 | 2:217:B:ARG:H    | 19       | 0.12          |
| (2,2122) | 2:207:B:VAL:HG23 | 2:217:B:ARG:H    | 19       | 0.12          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD11 | 20       | 0.12          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD12 | 20       | 0.12          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD13 | 20       | 0.12          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD21 | 20       | 0.12          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD22 | 20       | 0.12          |
| (2,2096) | 2:205:B:TRP:HZ2  | 2:218:B:LEU:HD23 | 20       | 0.12          |
| (2,2002) | 1:84:A:GLU:HA    | 1:87:A:ARG:HG2   | 7        | 0.12          |
| (2,2002) | 1:84:A:GLU:HA    | 1:87:A:ARG:HG3   | 7        | 0.12          |
| (2,1965) | 1:77:A:LEU:HD11  | 1:78:A:LYS:HB2   | 8        | 0.12          |
| (2,1965) | 1:77:A:LEU:HD12  | 1:78:A:LYS:HB2   | 8        | 0.12          |
| (2,1965) | 1:77:A:LEU:HD13  | 1:78:A:LYS:HB2   | 8        | 0.12          |
| (2,1965) | 1:77:A:LEU:HD21  | 1:78:A:LYS:HB2   | 8        | 0.12          |
| (2,1965) | 1:77:A:LEU:HD22  | 1:78:A:LYS:HB2   | 8        | 0.12          |
| (2,1965) | 1:77:A:LEU:HD23  | 1:78:A:LYS:HB2   | 8        | 0.12          |
| (2,1965) | 1:77:A:LEU:HD11  | 1:78:A:LYS:HB2   | 12       | 0.12          |
| (2,1965) | 1:77:A:LEU:HD12  | 1:78:A:LYS:HB2   | 12       | 0.12          |
| (2,1965) | 1:77:A:LEU:HD13  | 1:78:A:LYS:HB2   | 12       | 0.12          |
| (2,1965) | 1:77:A:LEU:HD21  | 1:78:A:LYS:HB2   | 12       | 0.12          |
| (2,1965) | 1:77:A:LEU:HD22  | 1:78:A:LYS:HB2   | 12       | 0.12          |
| (2,1965) | 1:77:A:LEU:HD23  | 1:78:A:LYS:HB2   | 12       | 0.12          |
| (2,1805) | 1:54:A:ILE:HG21  | 1:84:A:GLU:HB2   | 11       | 0.12          |
| (2,1805) | 1:54:A:ILE:HG21  | 1:84:A:GLU:HB3   | 11       | 0.12          |
| (2,1805) | 1:54:A:ILE:HG22  | 1:84:A:GLU:HB2   | 11       | 0.12          |
| (2,1805) | 1:54:A:ILE:HG22  | 1:84:A:GLU:HB3   | 11       | 0.12          |
| (2,1805) | 1:54:A:ILE:HG23  | 1:84:A:GLU:HB2   | 11       | 0.12          |
| (2,1805) | 1:54:A:ILE:HG23  | 1:84:A:GLU:HB3   | 11       | 0.12          |
| (2,1739) | 1:48:A:LEU:HD11  | 2:206:B:ARG:HA   | 2        | 0.12          |
| (2,1739) | 1:48:A:LEU:HD12  | 2:206:B:ARG:HA   | 2        | 0.12          |
| (2,1739) | 1:48:A:LEU:HD13  | 2:206:B:ARG:HA   | 2        | 0.12          |
| (2,1739) | 1:48:A:LEU:HD21  | 2:206:B:ARG:HA   | 2        | 0.12          |
| (2,1739) | 1:48:A:LEU:HD22  | 2:206:B:ARG:HA   | 2        | 0.12          |
| (2,1739) | 1:48:A:LEU:HD23  | 2:206:B:ARG:HA   | 2        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1691) | 1:41:A:ASN:HD21 | 2:207:B:VAL:HB   | 8        | 0.12          |
| (2,1691) | 1:41:A:ASN:HD22 | 2:207:B:VAL:HB   | 8        | 0.12          |
| (2,1686) | 1:41:A:ASN:HA   | 2:207:B:VAL:HG11 | 1        | 0.12          |
| (2,1686) | 1:41:A:ASN:HA   | 2:207:B:VAL:HG12 | 1        | 0.12          |
| (2,1686) | 1:41:A:ASN:HA   | 2:207:B:VAL:HG13 | 1        | 0.12          |
| (2,1686) | 1:41:A:ASN:HA   | 2:207:B:VAL:HG21 | 1        | 0.12          |
| (2,1686) | 1:41:A:ASN:HA   | 2:207:B:VAL:HG22 | 1        | 0.12          |
| (2,1686) | 1:41:A:ASN:HA   | 2:207:B:VAL:HG23 | 1        | 0.12          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB2   | 20       | 0.12          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB3   | 20       | 0.12          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB2   | 20       | 0.12          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB3   | 20       | 0.12          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD11  | 19       | 0.12          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD12  | 19       | 0.12          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD13  | 19       | 0.12          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD21  | 19       | 0.12          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD22  | 19       | 0.12          |
| (2,1619) | 1:35:A:GLN:HE21 | 1:38:A:LEU:HD23  | 19       | 0.12          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD11  | 19       | 0.12          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD12  | 19       | 0.12          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD13  | 19       | 0.12          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD21  | 19       | 0.12          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD22  | 19       | 0.12          |
| (2,1619) | 1:35:A:GLN:HE22 | 1:38:A:LEU:HD23  | 19       | 0.12          |
| (2,1609) | 1:35:A:GLN:H    | 1:38:A:LEU:HD11  | 2        | 0.12          |
| (2,1609) | 1:35:A:GLN:H    | 1:38:A:LEU:HD12  | 2        | 0.12          |
| (2,1609) | 1:35:A:GLN:H    | 1:38:A:LEU:HD13  | 2        | 0.12          |
| (2,1609) | 1:35:A:GLN:H    | 1:38:A:LEU:HD21  | 2        | 0.12          |
| (2,1609) | 1:35:A:GLN:H    | 1:38:A:LEU:HD22  | 2        | 0.12          |
| (2,1609) | 1:35:A:GLN:H    | 1:38:A:LEU:HD23  | 2        | 0.12          |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD11  | 17       | 0.12          |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD12  | 17       | 0.12          |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD13  | 17       | 0.12          |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD21  | 17       | 0.12          |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD22  | 17       | 0.12          |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD23  | 17       | 0.12          |
| (2,1604) | 1:34:A:ARG:HD3  | 1:38:A:LEU:HD11  | 17       | 0.12          |
| (2,1604) | 1:34:A:ARG:HD3  | 1:38:A:LEU:HD12  | 17       | 0.12          |
| (2,1604) | 1:34:A:ARG:HD3  | 1:38:A:LEU:HD13  | 17       | 0.12          |
| (2,1604) | 1:34:A:ARG:HD3  | 1:38:A:LEU:HD21  | 17       | 0.12          |
| (2,1604) | 1:34:A:ARG:HD3  | 1:38:A:LEU:HD22  | 17       | 0.12          |
| (2,1604) | 1:34:A:ARG:HD3  | 1:38:A:LEU:HD23  | 17       | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1527) | 1:26:A:LEU:HD11  | 1:27:A:PRO:HD2  | 4        | 0.12          |
| (2,1527) | 1:26:A:LEU:HD12  | 1:27:A:PRO:HD2  | 4        | 0.12          |
| (2,1527) | 1:26:A:LEU:HD13  | 1:27:A:PRO:HD2  | 4        | 0.12          |
| (2,1527) | 1:26:A:LEU:HD21  | 1:27:A:PRO:HD2  | 4        | 0.12          |
| (2,1527) | 1:26:A:LEU:HD22  | 1:27:A:PRO:HD2  | 4        | 0.12          |
| (2,1527) | 1:26:A:LEU:HD23  | 1:27:A:PRO:HD2  | 4        | 0.12          |
| (2,1526) | 1:26:A:LEU:HD11  | 1:27:A:PRO:HG2  | 11       | 0.12          |
| (2,1526) | 1:26:A:LEU:HD11  | 1:27:A:PRO:HG3  | 11       | 0.12          |
| (2,1526) | 1:26:A:LEU:HD12  | 1:27:A:PRO:HG2  | 11       | 0.12          |
| (2,1526) | 1:26:A:LEU:HD12  | 1:27:A:PRO:HG3  | 11       | 0.12          |
| (2,1526) | 1:26:A:LEU:HD13  | 1:27:A:PRO:HG2  | 11       | 0.12          |
| (2,1526) | 1:26:A:LEU:HD13  | 1:27:A:PRO:HG3  | 11       | 0.12          |
| (2,1526) | 1:26:A:LEU:HD21  | 1:27:A:PRO:HG2  | 11       | 0.12          |
| (2,1526) | 1:26:A:LEU:HD21  | 1:27:A:PRO:HG3  | 11       | 0.12          |
| (2,1526) | 1:26:A:LEU:HD22  | 1:27:A:PRO:HG2  | 11       | 0.12          |
| (2,1526) | 1:26:A:LEU:HD22  | 1:27:A:PRO:HG3  | 11       | 0.12          |
| (2,1526) | 1:26:A:LEU:HD23  | 1:27:A:PRO:HG2  | 11       | 0.12          |
| (2,1526) | 1:26:A:LEU:HD23  | 1:27:A:PRO:HG3  | 11       | 0.12          |
| (2,1471) | 1:74:A:PHE:H     | 2:215:B:LYS:H   | 8        | 0.12          |
| (2,1397) | 2:205:B:TRP:HB2  | 2:220:B:ARG:H   | 9        | 0.12          |
| (2,1388) | 2:213:B:PRO:HD2  | 2:214:B:LEU:H   | 9        | 0.12          |
| (2,1375) | 2:207:B:VAL:HA   | 2:219:B:THR:H   | 19       | 0.12          |
| (2,1357) | 2:205:B:TRP:H    | 2:205:B:TRP:HD1 | 19       | 0.12          |
| (2,1295) | 2:204:B:THR:HG21 | 2:205:B:TRP:H   | 16       | 0.12          |
| (2,1295) | 2:204:B:THR:HG22 | 2:205:B:TRP:H   | 16       | 0.12          |
| (2,1295) | 2:204:B:THR:HG23 | 2:205:B:TRP:H   | 16       | 0.12          |
| (2,1236) | 2:215:B:LYS:HB3  | 2:215:B:LYS:HE2 | 17       | 0.12          |
| (2,1236) | 2:215:B:LYS:HB3  | 2:215:B:LYS:HE2 | 18       | 0.12          |
| (2,1233) | 2:204:B:THR:HG21 | 2:205:B:TRP:HB3 | 9        | 0.12          |
| (2,1233) | 2:204:B:THR:HG22 | 2:205:B:TRP:HB3 | 9        | 0.12          |
| (2,1233) | 2:204:B:THR:HG23 | 2:205:B:TRP:HB3 | 9        | 0.12          |
| (2,1187) | 2:217:B:ARG:HG2  | 2:218:B:LEU:H   | 3        | 0.12          |
| (2,1102) | 1:75:A:GLU:H     | 2:215:B:LYS:HA  | 11       | 0.12          |
| (2,845)  | 1:71:A:GLU:H     | 1:71:A:GLU:HG3  | 8        | 0.12          |
| (2,496)  | 1:71:A:GLU:HG2   | 1:72:A:ILE:H    | 2        | 0.12          |
| (2,407)  | 1:52:A:VAL:HB    | 1:70:A:ILE:HG21 | 5        | 0.12          |
| (2,407)  | 1:52:A:VAL:HB    | 1:70:A:ILE:HG22 | 5        | 0.12          |
| (2,407)  | 1:52:A:VAL:HB    | 1:70:A:ILE:HG23 | 5        | 0.12          |
| (2,329)  | 1:39:A:ASP:HA    | 1:42:A:ARG:HG3  | 3        | 0.12          |
| (2,310)  | 1:37:A:SER:HA    | 1:40:A:ILE:HD11 | 2        | 0.12          |
| (2,310)  | 1:37:A:SER:HA    | 1:40:A:ILE:HD12 | 2        | 0.12          |
| (2,310)  | 1:37:A:SER:HA    | 1:40:A:ILE:HD13 | 2        | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,269)  | 1:31:A:ASP:HA    | 1:34:A:ARG:HB2  | 7        | 0.12          |
| (2,196)  | 1:39:A:ASP:HB2   | 1:93:A:LEU:HD11 | 10       | 0.12          |
| (2,196)  | 1:39:A:ASP:HB2   | 1:93:A:LEU:HD12 | 10       | 0.12          |
| (2,196)  | 1:39:A:ASP:HB2   | 1:93:A:LEU:HD13 | 10       | 0.12          |
| (2,108)  | 1:95:A:LYS:HA    | 1:96:A:LYS:H    | 9        | 0.12          |
| (2,3)    | 2:205:B:TRP:HE3  | 2:218:B:LEU:HB3 | 12       | 0.12          |
| (1,15)   | 1:52:A:VAL:O     | 1:56:A:GLN:N    | 20       | 0.12          |
| (1,13)   | 1:51:A:VAL:O     | 1:55:A:ILE:N    | 2        | 0.12          |
| (2,2201) | 2:215:B:LYS:H    | 2:215:B:LYS:HE2 | 20       | 0.11          |
| (2,2201) | 2:215:B:LYS:H    | 2:215:B:LYS:HE3 | 20       | 0.11          |
| (2,2199) | 2:214:B:LEU:HD11 | 2:215:B:LYS:H   | 12       | 0.11          |
| (2,2199) | 2:214:B:LEU:HD12 | 2:215:B:LYS:H   | 12       | 0.11          |
| (2,2199) | 2:214:B:LEU:HD13 | 2:215:B:LYS:H   | 12       | 0.11          |
| (2,2199) | 2:214:B:LEU:HD21 | 2:215:B:LYS:H   | 12       | 0.11          |
| (2,2199) | 2:214:B:LEU:HD22 | 2:215:B:LYS:H   | 12       | 0.11          |
| (2,2199) | 2:214:B:LEU:HD23 | 2:215:B:LYS:H   | 12       | 0.11          |
| (2,2169) | 2:210:B:SER:HB2  | 2:212:B:ASN:H   | 17       | 0.11          |
| (2,2169) | 2:210:B:SER:HB3  | 2:212:B:ASN:H   | 17       | 0.11          |
| (2,2127) | 2:207:B:VAL:HG11 | 2:218:B:LEU:HG  | 14       | 0.11          |
| (2,2127) | 2:207:B:VAL:HG12 | 2:218:B:LEU:HG  | 14       | 0.11          |
| (2,2127) | 2:207:B:VAL:HG13 | 2:218:B:LEU:HG  | 14       | 0.11          |
| (2,2127) | 2:207:B:VAL:HG21 | 2:218:B:LEU:HG  | 14       | 0.11          |
| (2,2127) | 2:207:B:VAL:HG22 | 2:218:B:LEU:HG  | 14       | 0.11          |
| (2,2127) | 2:207:B:VAL:HG23 | 2:218:B:LEU:HG  | 14       | 0.11          |
| (2,2123) | 2:207:B:VAL:HG11 | 2:217:B:ARG:HA  | 3        | 0.11          |
| (2,2123) | 2:207:B:VAL:HG12 | 2:217:B:ARG:HA  | 3        | 0.11          |
| (2,2123) | 2:207:B:VAL:HG13 | 2:217:B:ARG:HA  | 3        | 0.11          |
| (2,2123) | 2:207:B:VAL:HG21 | 2:217:B:ARG:HA  | 3        | 0.11          |
| (2,2123) | 2:207:B:VAL:HG22 | 2:217:B:ARG:HA  | 3        | 0.11          |
| (2,2123) | 2:207:B:VAL:HG23 | 2:217:B:ARG:HA  | 3        | 0.11          |
| (2,2068) | 1:95:A:LYS:H     | 1:96:A:LYS:HG2  | 3        | 0.11          |
| (2,2068) | 1:95:A:LYS:H     | 1:96:A:LYS:HG3  | 3        | 0.11          |
| (2,2001) | 1:84:A:GLU:HA    | 1:87:A:ARG:HB2  | 11       | 0.11          |
| (2,2001) | 1:84:A:GLU:HA    | 1:87:A:ARG:HB3  | 11       | 0.11          |
| (2,1965) | 1:77:A:LEU:HD11  | 1:78:A:LYS:HB2  | 7        | 0.11          |
| (2,1965) | 1:77:A:LEU:HD12  | 1:78:A:LYS:HB2  | 7        | 0.11          |
| (2,1965) | 1:77:A:LEU:HD13  | 1:78:A:LYS:HB2  | 7        | 0.11          |
| (2,1965) | 1:77:A:LEU:HD21  | 1:78:A:LYS:HB2  | 7        | 0.11          |
| (2,1965) | 1:77:A:LEU:HD22  | 1:78:A:LYS:HB2  | 7        | 0.11          |
| (2,1965) | 1:77:A:LEU:HD23  | 1:78:A:LYS:HB2  | 7        | 0.11          |
| (2,1965) | 1:77:A:LEU:HD11  | 1:78:A:LYS:HB2  | 14       | 0.11          |
| (2,1965) | 1:77:A:LEU:HD12  | 1:78:A:LYS:HB2  | 14       | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1965) | 1:77:A:LEU:HD13 | 1:78:A:LYS:HB2   | 14       | 0.11          |
| (2,1965) | 1:77:A:LEU:HD21 | 1:78:A:LYS:HB2   | 14       | 0.11          |
| (2,1965) | 1:77:A:LEU:HD22 | 1:78:A:LYS:HB2   | 14       | 0.11          |
| (2,1965) | 1:77:A:LEU:HD23 | 1:78:A:LYS:HB2   | 14       | 0.11          |
| (2,1953) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD11 | 12       | 0.11          |
| (2,1953) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD12 | 12       | 0.11          |
| (2,1953) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD13 | 12       | 0.11          |
| (2,1953) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD21 | 12       | 0.11          |
| (2,1953) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD22 | 12       | 0.11          |
| (2,1953) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD23 | 12       | 0.11          |
| (2,1942) | 1:74:A:PHE:HD1  | 1:82:A:LEU:HD11  | 17       | 0.11          |
| (2,1942) | 1:74:A:PHE:HD1  | 1:82:A:LEU:HD12  | 17       | 0.11          |
| (2,1942) | 1:74:A:PHE:HD1  | 1:82:A:LEU:HD13  | 17       | 0.11          |
| (2,1942) | 1:74:A:PHE:HD1  | 1:82:A:LEU:HD21  | 17       | 0.11          |
| (2,1942) | 1:74:A:PHE:HD1  | 1:82:A:LEU:HD22  | 17       | 0.11          |
| (2,1942) | 1:74:A:PHE:HD1  | 1:82:A:LEU:HD23  | 17       | 0.11          |
| (2,1942) | 1:74:A:PHE:HD2  | 1:82:A:LEU:HD11  | 17       | 0.11          |
| (2,1942) | 1:74:A:PHE:HD2  | 1:82:A:LEU:HD12  | 17       | 0.11          |
| (2,1942) | 1:74:A:PHE:HD2  | 1:82:A:LEU:HD13  | 17       | 0.11          |
| (2,1942) | 1:74:A:PHE:HD2  | 1:82:A:LEU:HD21  | 17       | 0.11          |
| (2,1942) | 1:74:A:PHE:HD2  | 1:82:A:LEU:HD22  | 17       | 0.11          |
| (2,1942) | 1:74:A:PHE:HD2  | 1:82:A:LEU:HD23  | 17       | 0.11          |
| (2,1926) | 1:73:A:ASP:HB2  | 1:76:A:THR:HG21  | 1        | 0.11          |
| (2,1926) | 1:73:A:ASP:HB2  | 1:76:A:THR:HG22  | 1        | 0.11          |
| (2,1926) | 1:73:A:ASP:HB2  | 1:76:A:THR:HG23  | 1        | 0.11          |
| (2,1926) | 1:73:A:ASP:HB3  | 1:76:A:THR:HG21  | 1        | 0.11          |
| (2,1926) | 1:73:A:ASP:HB3  | 1:76:A:THR:HG22  | 1        | 0.11          |
| (2,1926) | 1:73:A:ASP:HB3  | 1:76:A:THR:HG23  | 1        | 0.11          |
| (2,1926) | 1:73:A:ASP:HB2  | 1:76:A:THR:HG21  | 13       | 0.11          |
| (2,1926) | 1:73:A:ASP:HB2  | 1:76:A:THR:HG22  | 13       | 0.11          |
| (2,1926) | 1:73:A:ASP:HB2  | 1:76:A:THR:HG23  | 13       | 0.11          |
| (2,1926) | 1:73:A:ASP:HB3  | 1:76:A:THR:HG21  | 13       | 0.11          |
| (2,1926) | 1:73:A:ASP:HB3  | 1:76:A:THR:HG22  | 13       | 0.11          |
| (2,1926) | 1:73:A:ASP:HB3  | 1:76:A:THR:HG23  | 13       | 0.11          |
| (2,1903) | 1:68:A:ASP:HB3  | 2:220:B:ARG:HG2  | 4        | 0.11          |
| (2,1903) | 1:68:A:ASP:HB3  | 2:220:B:ARG:HG3  | 4        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG11 | 1:54:A:ILE:HD11  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG11 | 1:54:A:ILE:HD12  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG11 | 1:54:A:ILE:HD13  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG12 | 1:54:A:ILE:HD11  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG12 | 1:54:A:ILE:HD12  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG12 | 1:54:A:ILE:HD13  | 6        | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1766) | 1:51:A:VAL:HG13 | 1:54:A:ILE:HD11  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG13 | 1:54:A:ILE:HD12  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG13 | 1:54:A:ILE:HD13  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG21 | 1:54:A:ILE:HD11  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG21 | 1:54:A:ILE:HD12  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG21 | 1:54:A:ILE:HD13  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG22 | 1:54:A:ILE:HD11  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG22 | 1:54:A:ILE:HD12  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG22 | 1:54:A:ILE:HD13  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG23 | 1:54:A:ILE:HD11  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG23 | 1:54:A:ILE:HD12  | 6        | 0.11          |
| (2,1766) | 1:51:A:VAL:HG23 | 1:54:A:ILE:HD13  | 6        | 0.11          |
| (2,1736) | 1:48:A:LEU:HD11 | 2:205:B:TRP:H    | 13       | 0.11          |
| (2,1736) | 1:48:A:LEU:HD12 | 2:205:B:TRP:H    | 13       | 0.11          |
| (2,1736) | 1:48:A:LEU:HD13 | 2:205:B:TRP:H    | 13       | 0.11          |
| (2,1736) | 1:48:A:LEU:HD21 | 2:205:B:TRP:H    | 13       | 0.11          |
| (2,1736) | 1:48:A:LEU:HD22 | 2:205:B:TRP:H    | 13       | 0.11          |
| (2,1736) | 1:48:A:LEU:HD23 | 2:205:B:TRP:H    | 13       | 0.11          |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD11 | 5        | 0.11          |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD12 | 5        | 0.11          |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD13 | 5        | 0.11          |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD21 | 5        | 0.11          |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD22 | 5        | 0.11          |
| (2,1625) | 1:36:A:LEU:H    | 2:214:B:LEU:HD23 | 5        | 0.11          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB2   | 16       | 0.11          |
| (2,1621) | 1:35:A:GLN:HE21 | 1:39:A:ASP:HB3   | 16       | 0.11          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB2   | 16       | 0.11          |
| (2,1621) | 1:35:A:GLN:HE22 | 1:39:A:ASP:HB3   | 16       | 0.11          |
| (2,1609) | 1:35:A:GLN:H    | 1:38:A:LEU:HD11  | 9        | 0.11          |
| (2,1609) | 1:35:A:GLN:H    | 1:38:A:LEU:HD12  | 9        | 0.11          |
| (2,1609) | 1:35:A:GLN:H    | 1:38:A:LEU:HD13  | 9        | 0.11          |
| (2,1609) | 1:35:A:GLN:H    | 1:38:A:LEU:HD21  | 9        | 0.11          |
| (2,1609) | 1:35:A:GLN:H    | 1:38:A:LEU:HD22  | 9        | 0.11          |
| (2,1609) | 1:35:A:GLN:H    | 1:38:A:LEU:HD23  | 9        | 0.11          |
| (2,1606) | 1:34:A:ARG:HD2  | 2:213:B:PRO:HG3  | 17       | 0.11          |
| (2,1606) | 1:34:A:ARG:HD3  | 2:213:B:PRO:HG3  | 17       | 0.11          |
| (2,1605) | 1:34:A:ARG:HD2  | 2:213:B:PRO:HB2  | 13       | 0.11          |
| (2,1605) | 1:34:A:ARG:HD2  | 2:213:B:PRO:HB3  | 13       | 0.11          |
| (2,1605) | 1:34:A:ARG:HD3  | 2:213:B:PRO:HB2  | 13       | 0.11          |
| (2,1605) | 1:34:A:ARG:HD3  | 2:213:B:PRO:HB3  | 13       | 0.11          |
| (2,1532) | 1:28:A:MET:H    | 1:33:A:LYS:HD2   | 14       | 0.11          |
| (2,1532) | 1:28:A:MET:H    | 1:33:A:LYS:HD3   | 14       | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (2,1527) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HD2 | 9        | 0.11          |
| (2,1527) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HD2 | 9        | 0.11          |
| (2,1527) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HD2 | 9        | 0.11          |
| (2,1527) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HD2 | 9        | 0.11          |
| (2,1527) | 1:26:A:LEU:HD22 | 1:27:A:PRO:HD2 | 9        | 0.11          |
| (2,1527) | 1:26:A:LEU:HD23 | 1:27:A:PRO:HD2 | 9        | 0.11          |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG2 | 15       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG3 | 15       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HG2 | 15       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HG3 | 15       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HG2 | 15       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HG3 | 15       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HG2 | 15       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HG3 | 15       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD22 | 1:27:A:PRO:HG2 | 15       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD22 | 1:27:A:PRO:HG3 | 15       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD23 | 1:27:A:PRO:HG2 | 15       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD23 | 1:27:A:PRO:HG3 | 15       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG2 | 17       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG3 | 17       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HG2 | 17       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HG3 | 17       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HG2 | 17       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HG3 | 17       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HG2 | 17       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HG3 | 17       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD22 | 1:27:A:PRO:HG2 | 17       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD22 | 1:27:A:PRO:HG3 | 17       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD23 | 1:27:A:PRO:HG2 | 17       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD23 | 1:27:A:PRO:HG3 | 17       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG2 | 20       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG3 | 20       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HG2 | 20       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HG3 | 20       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HG2 | 20       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HG3 | 20       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HG2 | 20       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HG3 | 20       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD22 | 1:27:A:PRO:HG2 | 20       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD22 | 1:27:A:PRO:HG3 | 20       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD23 | 1:27:A:PRO:HG2 | 20       | 0.11          |
| (2,1526) | 1:26:A:LEU:HD23 | 1:27:A:PRO:HG3 | 20       | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1503) | 1:22:A:GLU:HB2  | 1:23:A:GLU:H     | 11       | 0.11          |
| (2,1503) | 1:22:A:GLU:HB3  | 1:23:A:GLU:H     | 11       | 0.11          |
| (2,1503) | 1:22:A:GLU:HB2  | 1:23:A:GLU:H     | 17       | 0.11          |
| (2,1503) | 1:22:A:GLU:HB3  | 1:23:A:GLU:H     | 17       | 0.11          |
| (2,1455) | 1:74:A:PHE:H    | 2:214:B:LEU:H    | 19       | 0.11          |
| (2,1415) | 1:70:A:ILE:HB   | 2:218:B:LEU:H    | 1        | 0.11          |
| (2,1406) | 2:214:B:LEU:HB2 | 2:215:B:LYS:H    | 5        | 0.11          |
| (2,1406) | 2:214:B:LEU:HB2 | 2:215:B:LYS:H    | 20       | 0.11          |
| (2,1386) | 2:204:B:THR:HB  | 2:205:B:TRP:H    | 15       | 0.11          |
| (2,1245) | 2:212:B:ASN:HB2 | 2:215:B:LYS:HG3  | 17       | 0.11          |
| (2,1163) | 2:205:B:TRP:HH2 | 2:218:B:LEU:HB3  | 5        | 0.11          |
| (2,969)  | 1:18:A:ASP:H    | 1:19:A:SER:HA    | 1        | 0.11          |
| (2,553)  | 1:27:A:PRO:HA   | 1:79:A:PRO:HB3   | 10       | 0.11          |
| (2,553)  | 1:27:A:PRO:HA   | 1:79:A:PRO:HB3   | 11       | 0.11          |
| (2,531)  | 1:76:A:THR:HG21 | 2:215:B:LYS:HD3  | 4        | 0.11          |
| (2,531)  | 1:76:A:THR:HG22 | 2:215:B:LYS:HD3  | 4        | 0.11          |
| (2,531)  | 1:76:A:THR:HG23 | 2:215:B:LYS:HD3  | 4        | 0.11          |
| (2,399)  | 1:50:A:ARG:HG3  | 1:53:A:HIS:HB2   | 14       | 0.11          |
| (2,349)  | 1:43:A:LEU:HD11 | 1:44:A:PRO:HD3   | 5        | 0.11          |
| (2,349)  | 1:43:A:LEU:HD12 | 1:44:A:PRO:HD3   | 5        | 0.11          |
| (2,349)  | 1:43:A:LEU:HD13 | 1:44:A:PRO:HD3   | 5        | 0.11          |
| (2,189)  | 1:70:A:ILE:HG12 | 2:205:B:TRP:HH2  | 5        | 0.11          |
| (2,68)   | 1:90:A:LYS:HA   | 1:93:A:LEU:HG    | 18       | 0.11          |
| (2,58)   | 1:76:A:THR:HG21 | 2:215:B:LYS:HG3  | 5        | 0.11          |
| (2,58)   | 1:76:A:THR:HG22 | 2:215:B:LYS:HG3  | 5        | 0.11          |
| (2,58)   | 1:76:A:THR:HG23 | 2:215:B:LYS:HG3  | 5        | 0.11          |
| (2,23)   | 1:70:A:ILE:HD11 | 2:205:B:TRP:HH2  | 9        | 0.11          |
| (2,23)   | 1:70:A:ILE:HD12 | 2:205:B:TRP:HH2  | 9        | 0.11          |
| (2,23)   | 1:70:A:ILE:HD13 | 2:205:B:TRP:HH2  | 9        | 0.11          |
| (1,21)   | 1:87:A:ARG:O    | 1:91:A:SER:N     | 16       | 0.11          |
| (1,21)   | 1:87:A:ARG:O    | 1:91:A:SER:N     | 18       | 0.11          |
| (2,1953) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD11 | 13       | 0.1           |
| (2,1953) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD12 | 13       | 0.1           |
| (2,1953) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD13 | 13       | 0.1           |
| (2,1953) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD21 | 13       | 0.1           |
| (2,1953) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD22 | 13       | 0.1           |
| (2,1953) | 1:75:A:GLU:HB3  | 2:214:B:LEU:HD23 | 13       | 0.1           |
| (2,1910) | 1:69:A:GLU:HG2  | 2:219:B:THR:HG21 | 19       | 0.1           |
| (2,1910) | 1:69:A:GLU:HG2  | 2:219:B:THR:HG22 | 19       | 0.1           |
| (2,1910) | 1:69:A:GLU:HG2  | 2:219:B:THR:HG23 | 19       | 0.1           |
| (2,1910) | 1:69:A:GLU:HG3  | 2:219:B:THR:HG21 | 19       | 0.1           |
| (2,1910) | 1:69:A:GLU:HG3  | 2:219:B:THR:HG22 | 19       | 0.1           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1910) | 1:69:A:GLU:HG3  | 2:219:B:THR:HG23 | 19       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD11 | 2:218:B:LEU:HD11 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD11 | 2:218:B:LEU:HD12 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD11 | 2:218:B:LEU:HD13 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD11 | 2:218:B:LEU:HD21 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD11 | 2:218:B:LEU:HD22 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD11 | 2:218:B:LEU:HD23 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD12 | 2:218:B:LEU:HD11 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD12 | 2:218:B:LEU:HD12 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD12 | 2:218:B:LEU:HD13 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD12 | 2:218:B:LEU:HD21 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD12 | 2:218:B:LEU:HD22 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD12 | 2:218:B:LEU:HD23 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD13 | 2:218:B:LEU:HD11 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD13 | 2:218:B:LEU:HD12 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD13 | 2:218:B:LEU:HD13 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD13 | 2:218:B:LEU:HD21 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD13 | 2:218:B:LEU:HD22 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD13 | 2:218:B:LEU:HD23 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD21 | 2:218:B:LEU:HD11 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD21 | 2:218:B:LEU:HD12 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD21 | 2:218:B:LEU:HD13 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD21 | 2:218:B:LEU:HD21 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD21 | 2:218:B:LEU:HD22 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD21 | 2:218:B:LEU:HD23 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD22 | 2:218:B:LEU:HD11 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD22 | 2:218:B:LEU:HD12 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD22 | 2:218:B:LEU:HD13 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD22 | 2:218:B:LEU:HD21 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD22 | 2:218:B:LEU:HD22 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD22 | 2:218:B:LEU:HD23 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD23 | 2:218:B:LEU:HD11 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD23 | 2:218:B:LEU:HD12 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD23 | 2:218:B:LEU:HD13 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD23 | 2:218:B:LEU:HD21 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD23 | 2:218:B:LEU:HD22 | 10       | 0.1           |
| (2,1745) | 1:48:A:LEU:HD23 | 2:218:B:LEU:HD23 | 10       | 0.1           |
| (2,1740) | 1:48:A:LEU:HD11 | 2:206:B:ARG:HB2  | 13       | 0.1           |
| (2,1740) | 1:48:A:LEU:HD11 | 2:206:B:ARG:HB3  | 13       | 0.1           |
| (2,1740) | 1:48:A:LEU:HD12 | 2:206:B:ARG:HB2  | 13       | 0.1           |
| (2,1740) | 1:48:A:LEU:HD12 | 2:206:B:ARG:HB3  | 13       | 0.1           |
| (2,1740) | 1:48:A:LEU:HD13 | 2:206:B:ARG:HB2  | 13       | 0.1           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1740) | 1:48:A:LEU:HD13 | 2:206:B:ARG:HB3  | 13       | 0.1           |
| (2,1740) | 1:48:A:LEU:HD21 | 2:206:B:ARG:HB2  | 13       | 0.1           |
| (2,1740) | 1:48:A:LEU:HD21 | 2:206:B:ARG:HB3  | 13       | 0.1           |
| (2,1740) | 1:48:A:LEU:HD22 | 2:206:B:ARG:HB2  | 13       | 0.1           |
| (2,1740) | 1:48:A:LEU:HD22 | 2:206:B:ARG:HB3  | 13       | 0.1           |
| (2,1740) | 1:48:A:LEU:HD23 | 2:206:B:ARG:HB2  | 13       | 0.1           |
| (2,1740) | 1:48:A:LEU:HD23 | 2:206:B:ARG:HB3  | 13       | 0.1           |
| (2,1686) | 1:41:A:ASN:HA   | 2:207:B:VAL:HG11 | 17       | 0.1           |
| (2,1686) | 1:41:A:ASN:HA   | 2:207:B:VAL:HG12 | 17       | 0.1           |
| (2,1686) | 1:41:A:ASN:HA   | 2:207:B:VAL:HG13 | 17       | 0.1           |
| (2,1686) | 1:41:A:ASN:HA   | 2:207:B:VAL:HG21 | 17       | 0.1           |
| (2,1686) | 1:41:A:ASN:HA   | 2:207:B:VAL:HG22 | 17       | 0.1           |
| (2,1686) | 1:41:A:ASN:HA   | 2:207:B:VAL:HG23 | 17       | 0.1           |
| (2,1670) | 1:39:A:ASP:HB2  | 1:89:A:VAL:HG11  | 10       | 0.1           |
| (2,1670) | 1:39:A:ASP:HB2  | 1:89:A:VAL:HG12  | 10       | 0.1           |
| (2,1670) | 1:39:A:ASP:HB2  | 1:89:A:VAL:HG13  | 10       | 0.1           |
| (2,1670) | 1:39:A:ASP:HB2  | 1:89:A:VAL:HG21  | 10       | 0.1           |
| (2,1670) | 1:39:A:ASP:HB2  | 1:89:A:VAL:HG22  | 10       | 0.1           |
| (2,1670) | 1:39:A:ASP:HB2  | 1:89:A:VAL:HG23  | 10       | 0.1           |
| (2,1670) | 1:39:A:ASP:HB3  | 1:89:A:VAL:HG11  | 10       | 0.1           |
| (2,1670) | 1:39:A:ASP:HB3  | 1:89:A:VAL:HG12  | 10       | 0.1           |
| (2,1670) | 1:39:A:ASP:HB3  | 1:89:A:VAL:HG13  | 10       | 0.1           |
| (2,1670) | 1:39:A:ASP:HB3  | 1:89:A:VAL:HG21  | 10       | 0.1           |
| (2,1670) | 1:39:A:ASP:HB3  | 1:89:A:VAL:HG22  | 10       | 0.1           |
| (2,1670) | 1:39:A:ASP:HB3  | 1:89:A:VAL:HG23  | 10       | 0.1           |
| (2,1644) | 1:36:A:LEU:HD11 | 1:85:A:LEU:HB2   | 3        | 0.1           |
| (2,1644) | 1:36:A:LEU:HD11 | 1:85:A:LEU:HB3   | 3        | 0.1           |
| (2,1644) | 1:36:A:LEU:HD12 | 1:85:A:LEU:HB2   | 3        | 0.1           |
| (2,1644) | 1:36:A:LEU:HD12 | 1:85:A:LEU:HB3   | 3        | 0.1           |
| (2,1644) | 1:36:A:LEU:HD13 | 1:85:A:LEU:HB2   | 3        | 0.1           |
| (2,1644) | 1:36:A:LEU:HD13 | 1:85:A:LEU:HB3   | 3        | 0.1           |
| (2,1644) | 1:36:A:LEU:HD21 | 1:85:A:LEU:HB2   | 3        | 0.1           |
| (2,1644) | 1:36:A:LEU:HD21 | 1:85:A:LEU:HB3   | 3        | 0.1           |
| (2,1644) | 1:36:A:LEU:HD22 | 1:85:A:LEU:HB2   | 3        | 0.1           |
| (2,1644) | 1:36:A:LEU:HD22 | 1:85:A:LEU:HB3   | 3        | 0.1           |
| (2,1644) | 1:36:A:LEU:HD23 | 1:85:A:LEU:HB2   | 3        | 0.1           |
| (2,1644) | 1:36:A:LEU:HD23 | 1:85:A:LEU:HB3   | 3        | 0.1           |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD11  | 20       | 0.1           |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD12  | 20       | 0.1           |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD13  | 20       | 0.1           |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD21  | 20       | 0.1           |
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD22  | 20       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1604) | 1:34:A:ARG:HD2  | 1:38:A:LEU:HD23 | 20       | 0.1           |
| (2,1604) | 1:34:A:ARG:HD3  | 1:38:A:LEU:HD11 | 20       | 0.1           |
| (2,1604) | 1:34:A:ARG:HD3  | 1:38:A:LEU:HD12 | 20       | 0.1           |
| (2,1604) | 1:34:A:ARG:HD3  | 1:38:A:LEU:HD13 | 20       | 0.1           |
| (2,1604) | 1:34:A:ARG:HD3  | 1:38:A:LEU:HD21 | 20       | 0.1           |
| (2,1604) | 1:34:A:ARG:HD3  | 1:38:A:LEU:HD22 | 20       | 0.1           |
| (2,1604) | 1:34:A:ARG:HD3  | 1:38:A:LEU:HD23 | 20       | 0.1           |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD11 | 1        | 0.1           |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD12 | 1        | 0.1           |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD13 | 1        | 0.1           |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD21 | 1        | 0.1           |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD22 | 1        | 0.1           |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD23 | 1        | 0.1           |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD11 | 7        | 0.1           |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD12 | 7        | 0.1           |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD13 | 7        | 0.1           |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD21 | 7        | 0.1           |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD22 | 7        | 0.1           |
| (2,1534) | 1:28:A:MET:H    | 1:82:A:LEU:HD23 | 7        | 0.1           |
| (2,1527) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HD2  | 20       | 0.1           |
| (2,1527) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HD2  | 20       | 0.1           |
| (2,1527) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HD2  | 20       | 0.1           |
| (2,1527) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HD2  | 20       | 0.1           |
| (2,1527) | 1:26:A:LEU:HD22 | 1:27:A:PRO:HD2  | 20       | 0.1           |
| (2,1527) | 1:26:A:LEU:HD23 | 1:27:A:PRO:HD2  | 20       | 0.1           |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG2  | 19       | 0.1           |
| (2,1526) | 1:26:A:LEU:HD11 | 1:27:A:PRO:HG3  | 19       | 0.1           |
| (2,1526) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HG2  | 19       | 0.1           |
| (2,1526) | 1:26:A:LEU:HD12 | 1:27:A:PRO:HG3  | 19       | 0.1           |
| (2,1526) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HG2  | 19       | 0.1           |
| (2,1526) | 1:26:A:LEU:HD13 | 1:27:A:PRO:HG3  | 19       | 0.1           |
| (2,1526) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HG2  | 19       | 0.1           |
| (2,1526) | 1:26:A:LEU:HD21 | 1:27:A:PRO:HG3  | 19       | 0.1           |
| (2,1526) | 1:26:A:LEU:HD22 | 1:27:A:PRO:HG2  | 19       | 0.1           |
| (2,1526) | 1:26:A:LEU:HD22 | 1:27:A:PRO:HG3  | 19       | 0.1           |
| (2,1526) | 1:26:A:LEU:HD23 | 1:27:A:PRO:HG2  | 19       | 0.1           |
| (2,1526) | 1:26:A:LEU:HD23 | 1:27:A:PRO:HG3  | 19       | 0.1           |
| (2,1460) | 2:210:B:SER:H   | 2:212:B:ASN:H   | 16       | 0.1           |
| (2,1451) | 1:71:A:GLU:HG3  | 2:218:B:LEU:H   | 7        | 0.1           |
| (2,1357) | 2:205:B:TRP:H   | 2:205:B:TRP:HD1 | 13       | 0.1           |
| (2,1353) | 1:74:A:PHE:HD1  | 2:215:B:LYS:H   | 18       | 0.1           |
| (2,1353) | 1:74:A:PHE:HD2  | 2:215:B:LYS:H   | 18       | 0.1           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1314) | 2:204:B:THR:HB  | 2:205:B:TRP:HA   | 18       | 0.1           |
| (2,1260) | 2:215:B:LYS:HB3 | 2:216:B:ILE:HG21 | 10       | 0.1           |
| (2,1260) | 2:215:B:LYS:HB3 | 2:216:B:ILE:HG22 | 10       | 0.1           |
| (2,1260) | 2:215:B:LYS:HB3 | 2:216:B:ILE:HG23 | 10       | 0.1           |
| (2,1102) | 1:75:A:GLU:H    | 2:215:B:LYS:HA   | 15       | 0.1           |
| (2,568)  | 1:28:A:MET:HE1  | 1:82:A:LEU:H     | 8        | 0.1           |
| (2,568)  | 1:28:A:MET:HE2  | 1:82:A:LEU:H     | 8        | 0.1           |
| (2,568)  | 1:28:A:MET:HE3  | 1:82:A:LEU:H     | 8        | 0.1           |
| (2,536)  | 1:74:A:PHE:HB2  | 2:214:B:LEU:HD11 | 7        | 0.1           |
| (2,536)  | 1:74:A:PHE:HB2  | 2:214:B:LEU:HD12 | 7        | 0.1           |
| (2,536)  | 1:74:A:PHE:HB2  | 2:214:B:LEU:HD13 | 7        | 0.1           |
| (2,496)  | 1:71:A:GLU:HG2  | 1:72:A:ILE:H     | 14       | 0.1           |
| (2,400)  | 1:50:A:ARG:HG3  | 1:53:A:HIS:HB3   | 20       | 0.1           |
| (1,20)   | 1:83:A:ARG:O    | 1:87:A:ARG:H     | 16       | 0.1           |
| (1,9)    | 1:49:A:GLY:O    | 1:53:A:HIS:N     | 5        | 0.1           |

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

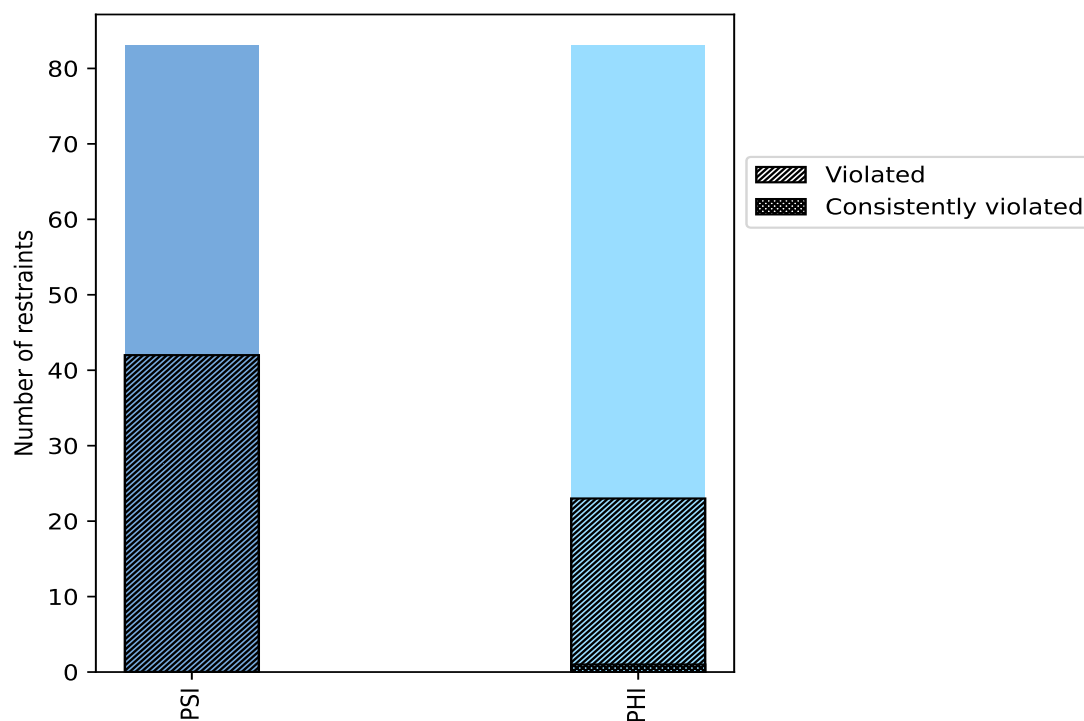
### 10.1 Summary of dihedral-angle violations [i](#)

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        | 83    | 50.0           | 42                    | 50.6           | 25.3           | 0                                  | 0.0            | 0.0            |
| PHI        | 83    | 50.0           | 23                    | 27.7           | 13.9           | 1                                  | 1.2            | 0.6            |
| Total      | 166   | 100.0          | 65                    | 39.2           | 39.2           | 1                                  | 0.6            | 0.6            |

<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](#)



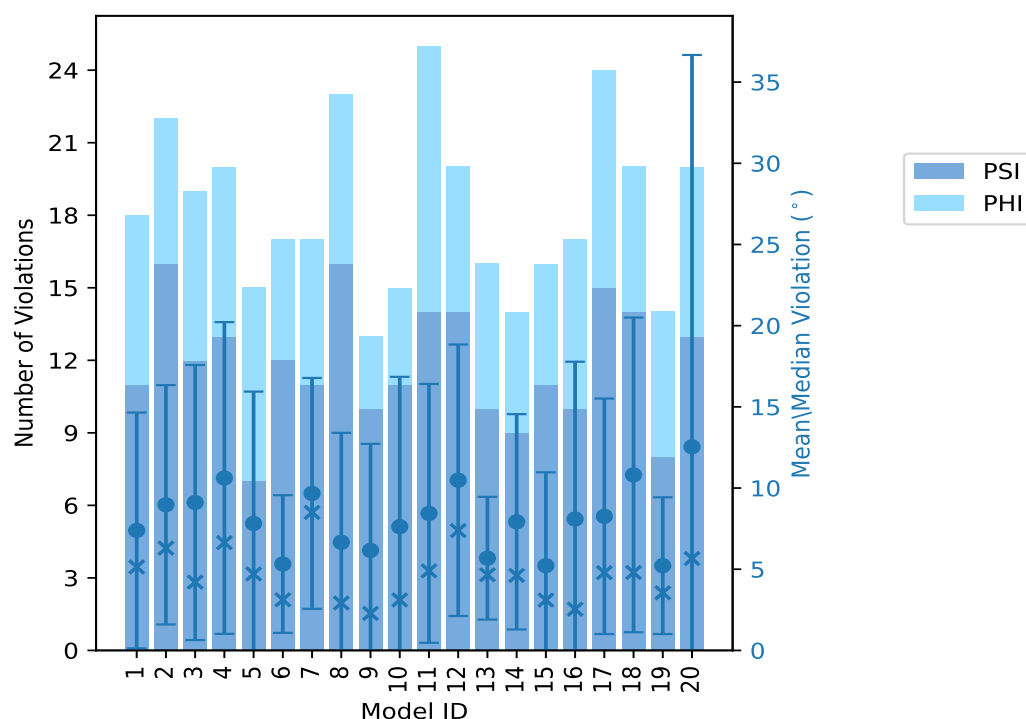
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model [i](#)

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        | 11                   | 7   | 18    | 7.39     | 30.36   | 7.26   | 5.14       |
| 2        | 16                   | 6   | 22    | 8.97     | 27.7    | 7.37   | 6.3        |
| 3        | 12                   | 7   | 19    | 9.11     | 24.9    | 8.47   | 4.21       |
| 4        | 13                   | 7   | 20    | 10.62    | 37.47   | 9.6    | 6.64       |
| 5        | 7                    | 8   | 15    | 7.82     | 26.86   | 8.12   | 4.71       |
| 6        | 12                   | 5   | 17    | 5.32     | 17.0    | 4.24   | 3.12       |
| 7        | 11                   | 6   | 17    | 9.67     | 21.48   | 7.11   | 8.5        |
| 8        | 16                   | 7   | 23    | 6.66     | 23.03   | 6.74   | 2.92       |
| 9        | 10                   | 3   | 13    | 6.16     | 21.76   | 6.56   | 2.28       |
| 10       | 11                   | 4   | 15    | 7.62     | 31.8    | 9.23   | 3.11       |
| 11       | 14                   | 11  | 25    | 8.44     | 25.58   | 7.97   | 4.9        |
| 12       | 14                   | 6   | 20    | 10.48    | 29.51   | 8.36   | 7.38       |
| 13       | 10                   | 6   | 16    | 5.68     | 15.0    | 3.78   | 4.66       |
| 14       | 9                    | 5   | 14    | 7.92     | 22.45   | 6.63   | 4.62       |
| 15       | 11                   | 5   | 16    | 5.22     | 20.72   | 5.75   | 3.1        |
| 16       | 10                   | 7   | 17    | 8.09     | 28.94   | 9.69   | 2.54       |
| 17       | 15                   | 9   | 24    | 8.26     | 27.55   | 7.25   | 4.79       |
| 18       | 14                   | 6   | 20    | 10.81    | 30.95   | 9.69   | 4.8        |
| 19       | 8                    | 6   | 14    | 5.22     | 18.36   | 4.21   | 3.55       |
| 20       | 13                   | 7   | 20    | 12.54    | 113.51  | 24.13  | 5.66       |

### 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>       | %    |
| 8                             | 6   | 14    | 1                        | 5.0  |
| 8                             | 1   | 9     | 2                        | 10.0 |
| 3                             | 6   | 9     | 3                        | 15.0 |
| 2                             | 1   | 3     | 4                        | 20.0 |
| 5                             | 1   | 6     | 5                        | 25.0 |
| 2                             | 2   | 4     | 6                        | 30.0 |
| 3                             | 0   | 3     | 7                        | 35.0 |
| 2                             | 2   | 4     | 8                        | 40.0 |
| 1                             | 0   | 1     | 9                        | 45.0 |
| 2                             | 0   | 2     | 10                       | 50.0 |
| 1                             | 1   | 2     | 11                       | 55.0 |

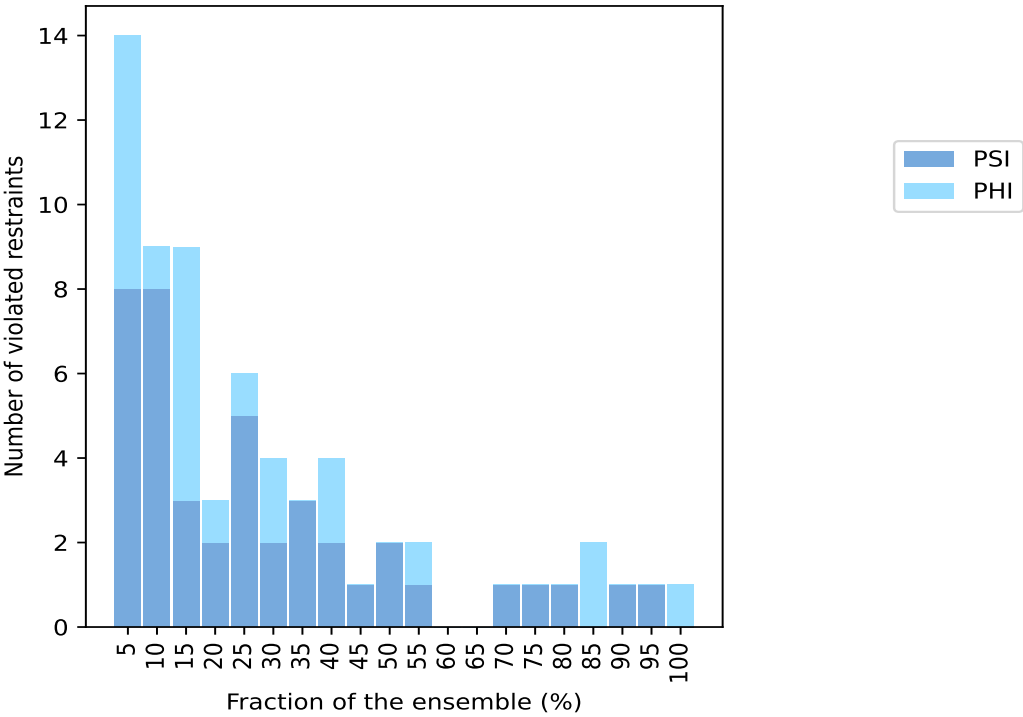
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |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

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

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

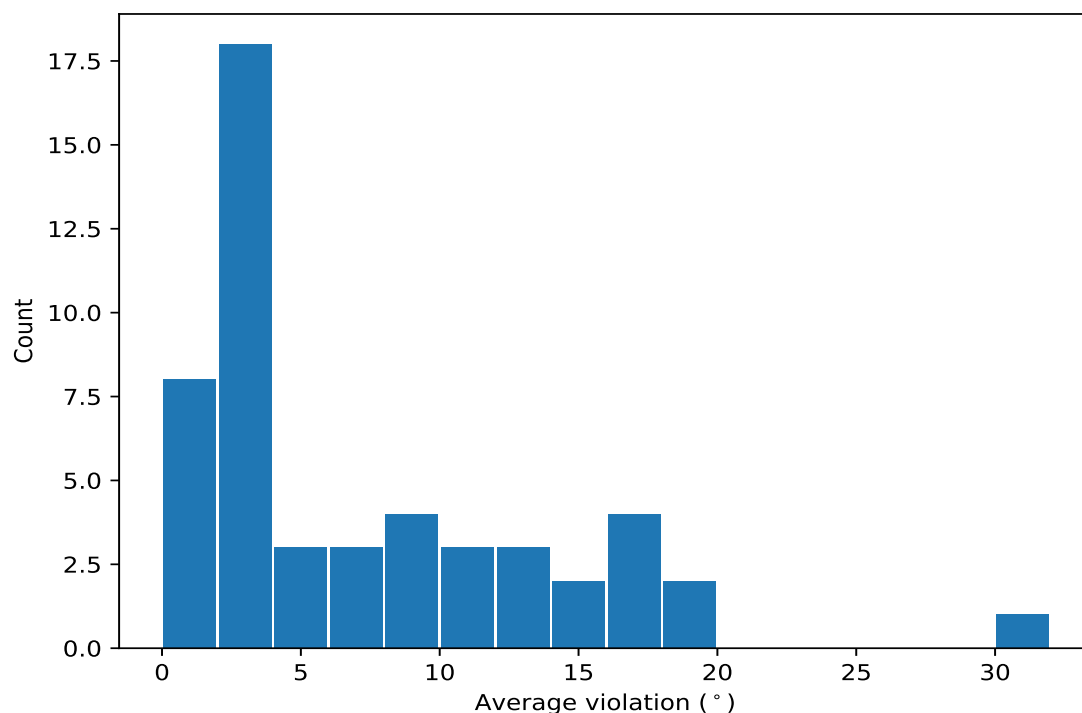


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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 |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 20                  | 14.44 | 8.04            | 13.09  |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 19                  | 16.55 | 5.66            | 18.96  |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 18                  | 3.0   | 1.52            | 2.61   |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 17                  | 16.38 | 6.0             | 16.7   |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 17                  | 9.47  | 5.48            | 8.26   |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 16                  | 3.82  | 1.69            | 3.78   |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 15                  | 3.77  | 1.63            | 3.18   |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 14                  | 2.69  | 1.4             | 2.24   |
| (1,154) | 2:216:B:ILE:N | 2:216:B:ILE:CA | 2:216:B:ILE:C  | 2:217:B:ARG:N | 11                  | 16.7  | 7.19            | 15.76  |
| (1,153) | 2:215:B:LYS:C | 2:216:B:ILE:N  | 2:216:B:ILE:CA | 2:216:B:ILE:C | 11                  | 11.93 | 8.26            | 13.14  |
| (1,152) | 2:215:B:LYS:N | 2:215:B:LYS:CA | 2:215:B:LYS:C  | 2:216:B:ILE:N | 10                  | 18.77 | 8.49            | 19.33  |
| (1,162) | 2:220:B:ARG:N | 2:220:B:ARG:CA | 2:220:B:ARG:C  | 2:221:B:GLU:N | 10                  | 8.45  | 2.86            | 8.95   |
| (1,166) | 2:222:B:ALA:N | 2:222:B:ALA:CA | 2:222:B:ALA:C  | 2:223:B:PRO:N | 9                   | 12.69 | 8.68            | 14.82  |
| (1,137) | 2:204:B:THR:C | 2:205:B:TRP:N  | 2:205:B:TRP:CA | 2:205:B:TRP:C | 8                   | 9.96  | 6.82            | 8.09   |
| (1,155) | 2:216:B:ILE:C | 2:217:B:ARG:N  | 2:217:B:ARG:CA | 2:217:B:ARG:C | 8                   | 8.04  | 4.37            | 6.66   |
| (1,82)  | 1:65:A:SER:N  | 1:65:A:SER:CA  | 1:65:A:SER:C   | 1:66:A:ASN:N  | 8                   | 2.57  | 0.88            | 2.34   |
| (1,12)  | 1:28:A:MET:N  | 1:28:A:MET:CA  | 1:28:A:MET:C   | 1:29:A:SER:N  | 8                   | 2.18  | 0.82            | 2.08   |
| (1,112) | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C   | 1:83:A:ARG:N  | 7                   | 2.6   | 1.14            | 2.56   |
| (1,92)  | 1:71:A:GLU:N  | 1:71:A:GLU:CA  | 1:71:A:GLU:C   | 1:72:A:ILE:N  | 7                   | 2.21  | 1.01            | 1.96   |
| (1,134) | 1:93:A:LEU:N  | 1:93:A:LEU:CA  | 1:93:A:LEU:C   | 1:94:A:GLN:N  | 7                   | 2.08  | 0.54            | 2.2    |

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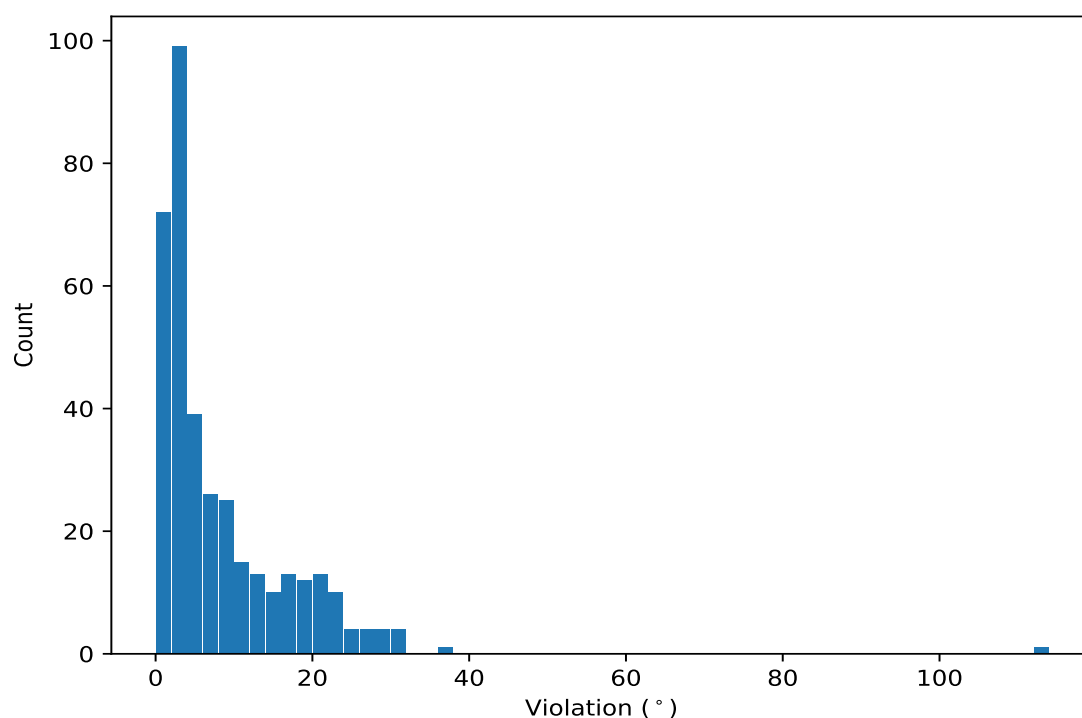
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,139) | 2:205:B:TRP:C | 2:206:B:ARG:N  | 2:206:B:ARG:CA | 2:206:B:ARG:C | 6                   | 11.6  | 7.99            | 7.97   |
| (1,156) | 2:217:B:ARG:N | 2:217:B:ARG:CA | 2:217:B:ARG:C  | 2:218:B:LEU:N | 6                   | 7.16  | 2.93            | 5.92   |
| (1,62)  | 1:54:A:ILE:N  | 1:54:A:ILE:CA  | 1:54:A:ILE:C   | 1:55:A:ILE:N  | 6                   | 2.72  | 0.76            | 2.56   |
| (1,35)  | 1:39:A:ASP:C  | 1:40:A:ILE:N   | 1:40:A:ILE:CA  | 1:40:A:ILE:C  | 6                   | 1.57  | 0.29            | 1.44   |
| (1,136) | 2:204:B:THR:N | 2:204:B:THR:CA | 2:204:B:THR:C  | 2:205:B:TRP:N | 5                   | 19.21 | 7.2             | 22.45  |
| (1,144) | 2:208:B:GLN:N | 2:208:B:GLN:CA | 2:208:B:GLN:C  | 2:209:B:ARG:N | 5                   | 16.14 | 5.51            | 14.68  |
| (1,142) | 2:207:B:VAL:N | 2:207:B:VAL:CA | 2:207:B:VAL:C  | 2:208:B:GLN:N | 5                   | 12.5  | 7.42            | 8.5    |
| (1,140) | 2:206:B:ARG:N | 2:206:B:ARG:CA | 2:206:B:ARG:C  | 2:207:B:VAL:N | 5                   | 6.33  | 5.43            | 4.8    |
| (1,135) | 2:203:B:LEU:C | 2:204:B:THR:N  | 2:204:B:THR:CA | 2:204:B:THR:C | 5                   | 5.18  | 4.44            | 2.31   |
| (1,66)  | 1:56:A:GLN:N  | 1:56:A:GLN:CA  | 1:56:A:GLN:C   | 1:57:A:SER:N  | 5                   | 2.62  | 0.63            | 2.64   |
| (1,164) | 2:221:B:GLU:N | 2:221:B:GLU:CA | 2:221:B:GLU:C  | 2:222:B:ALA:N | 4                   | 31.4  | 47.42           | 5.01   |
| (1,53)  | 1:49:A:GLY:C  | 1:50:A:ARG:N   | 1:50:A:ARG:CA  | 1:50:A:ARG:C  | 4                   | 1.76  | 0.55            | 1.76   |
| (1,46)  | 1:46:A:GLU:N  | 1:46:A:GLU:CA  | 1:46:A:GLU:C   | 1:47:A:LYS:N  | 4                   | 1.66  | 0.18            | 1.63   |
| (1,146) | 2:209:B:ARG:N | 2:209:B:ARG:CA | 2:209:B:ARG:C  | 2:210:B:SER:N | 3                   | 15.8  | 15.63           | 8.76   |
| (1,165) | 2:221:B:GLU:C | 2:222:B:ALA:N  | 2:222:B:ALA:CA | 2:222:B:ALA:C | 3                   | 13.82 | 12.54           | 7.34   |
| (1,160) | 2:219:B:THR:N | 2:219:B:THR:CA | 2:219:B:THR:C  | 2:220:B:ARG:N | 3                   | 6.69  | 2.29            | 6.95   |
| (1,149) | 2:211:B:GLN:C | 2:212:B:ASN:N  | 2:212:B:ASN:CA | 2:212:B:ASN:C | 3                   | 5.15  | 3.27            | 4.94   |
| (1,148) | 2:210:B:SER:N | 2:210:B:SER:CA | 2:210:B:SER:C  | 2:211:B:GLN:N | 3                   | 3.26  | 0.97            | 3.15   |
| (1,61)  | 1:53:A:HIS:C  | 1:54:A:ILE:N   | 1:54:A:ILE:CA  | 1:54:A:ILE:C  | 3                   | 2.96  | 0.59            | 3.17   |
| (1,3)   | 1:18:A:ASP:C  | 1:19:A:SER:N   | 1:19:A:SER:CA  | 1:19:A:SER:C  | 3                   | 2.67  | 1.16            | 3.43   |
| (1,83)  | 1:65:A:SER:C  | 1:66:A:ASN:N   | 1:66:A:ASN:CA  | 1:66:A:ASN:C  | 3                   | 1.64  | 0.14            | 1.73   |
| (1,31)  | 1:37:A:SER:C  | 1:38:A:LEU:N   | 1:38:A:LEU:CA  | 1:38:A:LEU:C  | 3                   | 1.61  | 0.12            | 1.64   |
| (1,138) | 2:205:B:TRP:N | 2:205:B:TRP:CA | 2:205:B:TRP:C  | 2:206:B:ARG:N | 2                   | 10.45 | 8.2             | 10.45  |
| (1,86)  | 1:68:A:ASP:N  | 1:68:A:ASP:CA  | 1:68:A:ASP:C   | 1:69:A:GLU:N  | 2                   | 4.38  | 0.76            | 4.38   |
| (1,34)  | 1:39:A:ASP:N  | 1:39:A:ASP:CA  | 1:39:A:ASP:C   | 1:40:A:ILE:N  | 2                   | 3.33  | 0.46            | 3.33   |
| (1,74)  | 1:61:A:SER:N  | 1:61:A:SER:CA  | 1:61:A:SER:C   | 1:62:A:LEU:N  | 2                   | 3.02  | 1.23            | 3.02   |
| (1,30)  | 1:37:A:SER:N  | 1:37:A:SER:CA  | 1:37:A:SER:C   | 1:38:A:LEU:N  | 2                   | 2.28  | 1.11            | 2.28   |
| (1,65)  | 1:55:A:ILE:C  | 1:56:A:GLN:N   | 1:56:A:GLN:CA  | 1:56:A:GLN:C  | 2                   | 2.06  | 0.68            | 2.06   |
| (1,64)  | 1:55:A:ILE:N  | 1:55:A:ILE:CA  | 1:55:A:ILE:C   | 1:56:A:GLN:N  | 2                   | 1.86  | 0.59            | 1.86   |
| (1,2)   | 1:18:A:ASP:N  | 1:18:A:ASP:CA  | 1:18:A:ASP:C   | 1:19:A:SER:N  | 2                   | 1.65  | 0.36            | 1.65   |
| (1,58)  | 1:52:A:VAL:N  | 1:52:A:VAL:CA  | 1:52:A:VAL:C   | 1:53:A:HIS:N  | 2                   | 1.52  | 0.5             | 1.52   |

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

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

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

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



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,164) | 2:221:B:GLU:N | 2:221:B:GLU:CA | 2:221:B:GLU:C  | 2:222:B:ALA:N | 20       | 113.51        |
| (1,146) | 2:209:B:ARG:N | 2:209:B:ARG:CA | 2:209:B:ARG:C  | 2:210:B:SER:N | 4        | 37.47         |
| (1,153) | 2:215:B:LYS:C | 2:216:B:ILE:N  | 2:216:B:ILE:CA | 2:216:B:ILE:C | 10       | 31.8          |
| (1,165) | 2:221:B:GLU:C | 2:222:B:ALA:N  | 2:222:B:ALA:CA | 2:222:B:ALA:C | 20       | 31.35         |
| (1,154) | 2:216:B:ILE:N | 2:216:B:ILE:CA | 2:216:B:ILE:C  | 2:217:B:ARG:N | 18       | 30.95         |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 1        | 30.36         |
| (1,152) | 2:215:B:LYS:N | 2:215:B:LYS:CA | 2:215:B:LYS:C  | 2:216:B:ILE:N | 12       | 29.51         |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 18       | 28.99         |
| (1,139) | 2:205:B:TRP:C | 2:206:B:ARG:N  | 2:206:B:ARG:CA | 2:206:B:ARG:C | 16       | 28.94         |
| (1,136) | 2:204:B:THR:N | 2:204:B:THR:CA | 2:204:B:THR:C  | 2:205:B:TRP:N | 16       | 28.55         |
| (1,166) | 2:222:B:ALA:N | 2:222:B:ALA:CA | 2:222:B:ALA:C  | 2:223:B:PRO:N | 2        | 27.7          |
| (1,152) | 2:215:B:LYS:N | 2:215:B:LYS:CA | 2:215:B:LYS:C  | 2:216:B:ILE:N | 17       | 27.55         |
| (1,144) | 2:208:B:GLN:N | 2:208:B:GLN:CA | 2:208:B:GLN:C  | 2:209:B:ARG:N | 5        | 26.86         |
| (1,152) | 2:215:B:LYS:N | 2:215:B:LYS:CA | 2:215:B:LYS:C  | 2:216:B:ILE:N | 10       | 26.6          |
| (1,152) | 2:215:B:LYS:N | 2:215:B:LYS:CA | 2:215:B:LYS:C  | 2:216:B:ILE:N | 11       | 25.58         |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 3        | 24.9          |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 11       | 24.8          |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 2        | 24.11         |
| (1,154) | 2:216:B:ILE:N | 2:216:B:ILE:CA | 2:216:B:ILE:C  | 2:217:B:ARG:N | 3        | 23.74         |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 5        | 23.33         |
| (1,154) | 2:216:B:ILE:N | 2:216:B:ILE:CA | 2:216:B:ILE:C  | 2:217:B:ARG:N | 17       | 23.23         |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,142) | 2:207:B:VAL:N | 2:207:B:VAL:CA | 2:207:B:VAL:C  | 2:208:B:GLN:N | 8        | 23.03         |
| (1,137) | 2:204:B:THR:C | 2:205:B:TRP:N  | 2:205:B:TRP:CA | 2:205:B:TRP:C | 11       | 22.66         |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 3        | 22.59         |
| (1,136) | 2:204:B:THR:N | 2:204:B:THR:CA | 2:204:B:THR:C  | 2:205:B:TRP:N | 8        | 22.53         |
| (1,136) | 2:204:B:THR:N | 2:204:B:THR:CA | 2:204:B:THR:C  | 2:205:B:TRP:N | 14       | 22.45         |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 11       | 22.18         |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 4        | 22.08         |
| (1,166) | 2:222:B:ALA:N | 2:222:B:ALA:CA | 2:222:B:ALA:C  | 2:223:B:PRO:N | 12       | 21.95         |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 4        | 21.84         |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 9        | 21.76         |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 3        | 21.61         |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 7        | 21.48         |
| (1,154) | 2:216:B:ILE:N | 2:216:B:ILE:CA | 2:216:B:ILE:C  | 2:217:B:ARG:N | 7        | 21.22         |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 18       | 21.2          |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 7        | 21.19         |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 12       | 21.02         |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 2        | 20.9          |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 16       | 20.9          |
| (1,152) | 2:215:B:LYS:N | 2:215:B:LYS:CA | 2:215:B:LYS:C  | 2:216:B:ILE:N | 18       | 20.89         |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 15       | 20.72         |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 4        | 19.91         |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 12       | 19.8          |
| (1,142) | 2:207:B:VAL:N | 2:207:B:VAL:CA | 2:207:B:VAL:C  | 2:208:B:GLN:N | 18       | 19.72         |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 1        | 19.61         |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 4        | 19.52         |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 12       | 19.24         |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 15       | 18.96         |
| (1,137) | 2:204:B:THR:C | 2:205:B:TRP:N  | 2:205:B:TRP:CA | 2:205:B:TRP:C | 18       | 18.87         |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 14       | 18.69         |
| (1,138) | 2:205:B:TRP:N | 2:205:B:TRP:CA | 2:205:B:TRP:C  | 2:206:B:ARG:N | 16       | 18.65         |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 19       | 18.36         |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 9        | 18.16         |
| (1,154) | 2:216:B:ILE:N | 2:216:B:ILE:CA | 2:216:B:ILE:C  | 2:217:B:ARG:N | 12       | 17.94         |
| (1,152) | 2:215:B:LYS:N | 2:215:B:LYS:CA | 2:215:B:LYS:C  | 2:216:B:ILE:N | 7        | 17.76         |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 14       | 17.52         |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 5        | 17.19         |
| (1,166) | 2:222:B:ALA:N | 2:222:B:ALA:CA | 2:222:B:ALA:C  | 2:223:B:PRO:N | 3        | 17.18         |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 6        | 17.0          |
| (1,153) | 2:215:B:LYS:C | 2:216:B:ILE:N  | 2:216:B:ILE:CA | 2:216:B:ILE:C | 17       | 16.89         |
| (1,166) | 2:222:B:ALA:N | 2:222:B:ALA:CA | 2:222:B:ALA:C  | 2:223:B:PRO:N | 18       | 16.75         |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 2        | 16.7          |
| (1,140) | 2:206:B:ARG:N | 2:206:B:ARG:CA | 2:206:B:ARG:C  | 2:207:B:VAL:N | 2        | 16.64         |
| (1,155) | 2:216:B:ILE:C | 2:217:B:ARG:N  | 2:217:B:ARG:CA | 2:217:B:ARG:C | 3        | 16.59         |
| (1,152) | 2:215:B:LYS:N | 2:215:B:LYS:CA | 2:215:B:LYS:C  | 2:216:B:ILE:N | 4        | 16.56         |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 8        | 16.55         |
| (1,153) | 2:215:B:LYS:C | 2:216:B:ILE:N  | 2:216:B:ILE:CA | 2:216:B:ILE:C | 11       | 15.92         |
| (1,154) | 2:216:B:ILE:N | 2:216:B:ILE:CA | 2:216:B:ILE:C  | 2:217:B:ARG:N | 8        | 15.76         |
| (1,153) | 2:215:B:LYS:C | 2:216:B:ILE:N  | 2:216:B:ILE:CA | 2:216:B:ILE:C | 7        | 15.4          |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 17       | 15.29         |
| (1,144) | 2:208:B:GLN:N | 2:208:B:GLN:CA | 2:208:B:GLN:C  | 2:209:B:ARG:N | 13       | 15.0          |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 17       | 14.88         |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,166) | 2:222:B:ALA:N | 2:222:B:ALA:CA | 2:222:B:ALA:C  | 2:223:B:PRO:N | 4        | 14.82         |
| (1,136) | 2:204:B:THR:N | 2:204:B:THR:CA | 2:204:B:THR:C  | 2:205:B:TRP:N | 20       | 14.7          |
| (1,144) | 2:208:B:GLN:N | 2:208:B:GLN:CA | 2:208:B:GLN:C  | 2:209:B:ARG:N | 17       | 14.68         |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 18       | 14.36         |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 10       | 13.83         |
| (1,155) | 2:216:B:ILE:C | 2:217:B:ARG:N  | 2:217:B:ARG:CA | 2:217:B:ARG:C | 18       | 13.83         |
| (1,162) | 2:220:B:ARG:N | 2:220:B:ARG:CA | 2:220:B:ARG:C  | 2:221:B:GLU:N | 17       | 13.67         |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 16       | 13.36         |
| (1,153) | 2:215:B:LYS:C | 2:216:B:ILE:N  | 2:216:B:ILE:CA | 2:216:B:ILE:C | 12       | 13.28         |
| (1,154) | 2:216:B:ILE:N | 2:216:B:ILE:CA | 2:216:B:ILE:C  | 2:217:B:ARG:N | 11       | 13.24         |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 20       | 13.16         |
| (1,153) | 2:215:B:LYS:C | 2:216:B:ILE:N  | 2:216:B:ILE:CA | 2:216:B:ILE:C | 4        | 13.14         |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 5        | 12.82         |
| (1,154) | 2:216:B:ILE:N | 2:216:B:ILE:CA | 2:216:B:ILE:C  | 2:217:B:ARG:N | 1        | 12.72         |
| (1,144) | 2:208:B:GLN:N | 2:208:B:GLN:CA | 2:208:B:GLN:C  | 2:209:B:ARG:N | 12       | 12.55         |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 12       | 12.31         |
| (1,139) | 2:205:B:TRP:C | 2:206:B:ARG:N  | 2:206:B:ARG:CA | 2:206:B:ARG:C | 11       | 12.1          |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 8        | 11.9          |
| (1,135) | 2:203:B:LEU:C | 2:204:B:THR:N  | 2:204:B:THR:CA | 2:204:B:THR:C | 17       | 11.86         |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 10       | 11.75         |
| (1,152) | 2:215:B:LYS:N | 2:215:B:LYS:CA | 2:215:B:LYS:C  | 2:216:B:ILE:N | 2        | 11.69         |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 11       | 11.67         |
| (1,144) | 2:208:B:GLN:N | 2:208:B:GLN:CA | 2:208:B:GLN:C  | 2:209:B:ARG:N | 11       | 11.62         |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 7        | 11.58         |
| (1,162) | 2:220:B:ARG:N | 2:220:B:ARG:CA | 2:220:B:ARG:C  | 2:221:B:GLU:N | 8        | 11.28         |
| (1,156) | 2:217:B:ARG:N | 2:217:B:ARG:CA | 2:217:B:ARG:C  | 2:218:B:LEU:N | 4        | 11.27         |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 6        | 11.23         |
| (1,156) | 2:217:B:ARG:N | 2:217:B:ARG:CA | 2:217:B:ARG:C  | 2:218:B:LEU:N | 7        | 11.05         |
| (1,137) | 2:204:B:THR:C | 2:205:B:TRP:N  | 2:205:B:TRP:CA | 2:205:B:TRP:C | 13       | 10.9          |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 20       | 10.63         |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 14       | 10.36         |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 17       | 10.1          |
| (1,154) | 2:216:B:ILE:N | 2:216:B:ILE:CA | 2:216:B:ILE:C  | 2:217:B:ARG:N | 6        | 9.92          |
| (1,153) | 2:215:B:LYS:C | 2:216:B:ILE:N  | 2:216:B:ILE:CA | 2:216:B:ILE:C | 13       | 9.9           |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 7        | 9.84          |
| (1,162) | 2:220:B:ARG:N | 2:220:B:ARG:CA | 2:220:B:ARG:C  | 2:221:B:GLU:N | 11       | 9.77          |
| (1,162) | 2:220:B:ARG:N | 2:220:B:ARG:CA | 2:220:B:ARG:C  | 2:221:B:GLU:N | 19       | 9.48          |
| (1,160) | 2:219:B:THR:N | 2:219:B:THR:CA | 2:219:B:THR:C  | 2:220:B:ARG:N | 2        | 9.36          |
| (1,137) | 2:204:B:THR:C | 2:205:B:TRP:N  | 2:205:B:TRP:CA | 2:205:B:TRP:C | 8        | 9.32          |
| (1,154) | 2:216:B:ILE:N | 2:216:B:ILE:CA | 2:216:B:ILE:C  | 2:217:B:ARG:N | 20       | 9.3           |
| (1,162) | 2:220:B:ARG:N | 2:220:B:ARG:CA | 2:220:B:ARG:C  | 2:221:B:GLU:N | 20       | 9.29          |
| (1,149) | 2:211:B:GLN:C | 2:212:B:ASN:N  | 2:212:B:ASN:CA | 2:212:B:ASN:C | 1        | 9.26          |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 1        | 9.18          |
| (1,135) | 2:203:B:LEU:C | 2:204:B:THR:N  | 2:204:B:THR:CA | 2:204:B:THR:C | 1        | 9.13          |
| (1,152) | 2:215:B:LYS:N | 2:215:B:LYS:CA | 2:215:B:LYS:C  | 2:216:B:ILE:N | 20       | 9.03          |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 9        | 8.98          |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 14       | 8.83          |
| (1,146) | 2:209:B:ARG:N | 2:209:B:ARG:CA | 2:209:B:ARG:C  | 2:210:B:SER:N | 9        | 8.76          |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 13       | 8.75          |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 6        | 8.65          |
| (1,162) | 2:220:B:ARG:N | 2:220:B:ARG:CA | 2:220:B:ARG:C  | 2:221:B:GLU:N | 1        | 8.61          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,142) | 2:207:B:VAL:N | 2:207:B:VAL:CA | 2:207:B:VAL:C  | 2:208:B:GLN:N | 7        | 8.5           |
| (1,139) | 2:205:B:TRP:C | 2:206:B:ARG:N  | 2:206:B:ARG:CA | 2:206:B:ARG:C | 6        | 8.34          |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 13       | 8.31          |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 2        | 8.26          |
| (1,162) | 2:220:B:ARG:N | 2:220:B:ARG:CA | 2:220:B:ARG:C  | 2:221:B:GLU:N | 12       | 8.05          |
| (1,153) | 2:215:B:LYS:C | 2:216:B:ILE:N  | 2:216:B:ILE:CA | 2:216:B:ILE:C | 2        | 8.04          |
| (1,136) | 2:204:B:THR:N | 2:204:B:THR:CA | 2:204:B:THR:C  | 2:205:B:TRP:N | 9        | 7.81          |
| (1,139) | 2:205:B:TRP:C | 2:206:B:ARG:N  | 2:206:B:ARG:CA | 2:206:B:ARG:C | 14       | 7.6           |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 19       | 7.49          |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 15       | 7.43          |
| (1,166) | 2:222:B:ALA:N | 2:222:B:ALA:CA | 2:222:B:ALA:C  | 2:223:B:PRO:N | 5        | 7.41          |
| (1,165) | 2:221:B:GLU:C | 2:222:B:ALA:N  | 2:222:B:ALA:CA | 2:222:B:ALA:C | 4        | 7.34          |
| (1,155) | 2:216:B:ILE:C | 2:217:B:ARG:N  | 2:217:B:ARG:CA | 2:217:B:ARG:C | 17       | 7.2           |
| (1,157) | 2:217:B:ARG:C | 2:218:B:LEU:N  | 2:218:B:LEU:CA | 2:218:B:LEU:C | 16       | 7.13          |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 3        | 7.11          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 2        | 7.01          |
| (1,155) | 2:216:B:ILE:C | 2:217:B:ARG:N  | 2:217:B:ARG:CA | 2:217:B:ARG:C | 7        | 6.96          |
| (1,160) | 2:219:B:THR:N | 2:219:B:THR:CA | 2:219:B:THR:C  | 2:220:B:ARG:N | 3        | 6.95          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 2        | 6.95          |
| (1,137) | 2:204:B:THR:C | 2:205:B:TRP:N  | 2:205:B:TRP:CA | 2:205:B:TRP:C | 20       | 6.86          |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 17       | 6.74          |
| (1,156) | 2:217:B:ARG:N | 2:217:B:ARG:CA | 2:217:B:ARG:C  | 2:218:B:LEU:N | 12       | 6.72          |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 6        | 6.62          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 5        | 6.59          |
| (1,142) | 2:207:B:VAL:N | 2:207:B:VAL:CA | 2:207:B:VAL:C  | 2:208:B:GLN:N | 12       | 6.46          |
| (1,139) | 2:205:B:TRP:C | 2:206:B:ARG:N  | 2:206:B:ARG:CA | 2:206:B:ARG:C | 8        | 6.46          |
| (1,155) | 2:216:B:ILE:C | 2:217:B:ARG:N  | 2:217:B:ARG:CA | 2:217:B:ARG:C | 12       | 6.37          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 1        | 6.37          |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 19       | 6.25          |
| (1,140) | 2:206:B:ARG:N | 2:206:B:ARG:CA | 2:206:B:ARG:C  | 2:207:B:VAL:N | 11       | 6.23          |
| (1,139) | 2:205:B:TRP:C | 2:206:B:ARG:N  | 2:206:B:ARG:CA | 2:206:B:ARG:C | 20       | 6.17          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 5        | 6.06          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 4        | 5.94          |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 13       | 5.91          |
| (1,162) | 2:220:B:ARG:N | 2:220:B:ARG:CA | 2:220:B:ARG:C  | 2:221:B:GLU:N | 3        | 5.82          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 15       | 5.72          |
| (1,154) | 2:216:B:ILE:N | 2:216:B:ILE:CA | 2:216:B:ILE:C  | 2:217:B:ARG:N | 2        | 5.65          |
| (1,164) | 2:221:B:GLU:N | 2:221:B:GLU:CA | 2:221:B:GLU:C  | 2:222:B:ALA:N | 2        | 5.52          |
| (1,155) | 2:216:B:ILE:C | 2:217:B:ARG:N  | 2:217:B:ARG:CA | 2:217:B:ARG:C | 1        | 5.5           |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 13       | 5.47          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 13       | 5.26          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 10       | 5.17          |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 20       | 5.16          |
| (1,86)  | 1:68:A:ASP:N  | 1:68:A:ASP:CA  | 1:68:A:ASP:C   | 1:69:A:GLU:N  | 2        | 5.14          |
| (1,156) | 2:217:B:ARG:N | 2:217:B:ARG:CA | 2:217:B:ARG:C  | 2:218:B:LEU:N | 17       | 5.13          |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 18       | 5.02          |
| (1,149) | 2:211:B:GLN:C | 2:212:B:ASN:N  | 2:212:B:ASN:CA | 2:212:B:ASN:C | 11       | 4.94          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 11       | 4.9           |
| (1,162) | 2:220:B:ARG:N | 2:220:B:ARG:CA | 2:220:B:ARG:C  | 2:221:B:GLU:N | 2        | 4.85          |
| (1,140) | 2:206:B:ARG:N | 2:206:B:ARG:CA | 2:206:B:ARG:C  | 2:207:B:VAL:N | 4        | 4.8           |
| (1,155) | 2:216:B:ILE:C | 2:217:B:ARG:N  | 2:217:B:ARG:CA | 2:217:B:ARG:C | 19       | 4.79          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,142) | 2:207:B:VAL:N | 2:207:B:VAL:CA | 2:207:B:VAL:C  | 2:208:B:GLN:N | 10       | 4.79          |
| (1,112) | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C   | 1:83:A:ARG:N  | 1        | 4.79          |
| (1,137) | 2:204:B:THR:C | 2:205:B:TRP:N  | 2:205:B:TRP:CA | 2:205:B:TRP:C | 14       | 4.71          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 5        | 4.71          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 7        | 4.67          |
| (1,166) | 2:222:B:ALA:N | 2:222:B:ALA:CA | 2:222:B:ALA:C  | 2:223:B:PRO:N | 8        | 4.61          |
| (1,156) | 2:217:B:ARG:N | 2:217:B:ARG:CA | 2:217:B:ARG:C  | 2:218:B:LEU:N | 18       | 4.59          |
| (1,92)  | 1:71:A:GLU:N  | 1:71:A:GLU:CA  | 1:71:A:GLU:C   | 1:72:A:ILE:N  | 14       | 4.53          |
| (1,164) | 2:221:B:GLU:N | 2:221:B:GLU:CA | 2:221:B:GLU:C  | 2:222:B:ALA:N | 8        | 4.51          |
| (1,148) | 2:210:B:SER:N | 2:210:B:SER:CA | 2:210:B:SER:C  | 2:211:B:GLN:N | 18       | 4.5           |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 17       | 4.45          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 12       | 4.41          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 6        | 4.35          |
| (1,74)  | 1:61:A:SER:N  | 1:61:A:SER:CA  | 1:61:A:SER:C   | 1:62:A:LEU:N  | 11       | 4.26          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 6        | 4.25          |
| (1,156) | 2:217:B:ARG:N | 2:217:B:ARG:CA | 2:217:B:ARG:C  | 2:218:B:LEU:N | 3        | 4.21          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 20       | 4.09          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 13       | 4.07          |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 17       | 4.01          |
| (1,62)  | 1:54:A:ILE:N  | 1:54:A:ILE:CA  | 1:54:A:ILE:C   | 1:55:A:ILE:N  | 15       | 4.0           |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 7        | 3.98          |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 18       | 3.96          |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 8        | 3.92          |
| (1,34)  | 1:39:A:ASP:N  | 1:39:A:ASP:CA  | 1:39:A:ASP:C   | 1:40:A:ILE:N  | 14       | 3.79          |
| (1,137) | 2:204:B:THR:C | 2:205:B:TRP:N  | 2:205:B:TRP:CA | 2:205:B:TRP:C | 2        | 3.77          |
| (1,160) | 2:219:B:THR:N | 2:219:B:THR:CA | 2:219:B:THR:C  | 2:220:B:ARG:N | 4        | 3.76          |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 2        | 3.76          |
| (1,82)  | 1:65:A:SER:N  | 1:65:A:SER:CA  | 1:65:A:SER:C   | 1:66:A:ASN:N  | 15       | 3.7           |
| (1,162) | 2:220:B:ARG:N | 2:220:B:ARG:CA | 2:220:B:ARG:C  | 2:221:B:GLU:N | 13       | 3.64          |
| (1,86)  | 1:68:A:ASP:N  | 1:68:A:ASP:CA  | 1:68:A:ASP:C   | 1:69:A:GLU:N  | 1        | 3.61          |
| (1,82)  | 1:65:A:SER:N  | 1:65:A:SER:CA  | 1:65:A:SER:C   | 1:66:A:ASN:N  | 19       | 3.59          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 19       | 3.57          |
| (1,3)   | 1:18:A:ASP:C  | 1:19:A:SER:N   | 1:19:A:SER:CA  | 1:19:A:SER:C  | 15       | 3.56          |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 11       | 3.55          |
| (1,82)  | 1:65:A:SER:N  | 1:65:A:SER:CA  | 1:65:A:SER:C   | 1:66:A:ASN:N  | 7        | 3.55          |
| (1,61)  | 1:53:A:HIS:C  | 1:54:A:ILE:N   | 1:54:A:ILE:CA  | 1:54:A:ILE:C  | 10       | 3.55          |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 19       | 3.53          |
| (1,153) | 2:215:B:LYS:C | 2:216:B:ILE:N  | 2:216:B:ILE:CA | 2:216:B:ILE:C | 19       | 3.52          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 17       | 3.46          |
| (1,66)  | 1:56:A:GLN:N  | 1:56:A:GLN:CA  | 1:56:A:GLN:C   | 1:57:A:SER:N  | 13       | 3.46          |
| (1,3)   | 1:18:A:ASP:C  | 1:19:A:SER:N   | 1:19:A:SER:CA  | 1:19:A:SER:C  | 17       | 3.43          |
| (1,30)  | 1:37:A:SER:N  | 1:37:A:SER:CA  | 1:37:A:SER:C   | 1:38:A:LEU:N  | 9        | 3.39          |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 4        | 3.37          |
| (1,128) | 1:90:A:LYS:N  | 1:90:A:LYS:CA  | 1:90:A:LYS:C   | 1:91:A:SER:N  | 15       | 3.34          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 14       | 3.28          |
| (1,62)  | 1:54:A:ILE:N  | 1:54:A:ILE:CA  | 1:54:A:ILE:C   | 1:55:A:ILE:N  | 20       | 3.23          |
| (1,12)  | 1:28:A:MET:N  | 1:28:A:MET:CA  | 1:28:A:MET:C   | 1:29:A:SER:N  | 19       | 3.22          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 3        | 3.18          |
| (1,61)  | 1:53:A:HIS:C  | 1:54:A:ILE:N   | 1:54:A:ILE:CA  | 1:54:A:ILE:C  | 3        | 3.17          |
| (1,148) | 2:210:B:SER:N | 2:210:B:SER:CA | 2:210:B:SER:C  | 2:211:B:GLN:N | 11       | 3.15          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 19       | 3.15          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,12)  | 1:28:A:MET:N  | 1:28:A:MET:CA  | 1:28:A:MET:C   | 1:29:A:SER:N  | 2        | 3.14          |
| (1,155) | 2:216:B:ILE:C | 2:217:B:ARG:N  | 2:217:B:ARG:CA | 2:217:B:ARG:C | 6        | 3.12          |
| (1,112) | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C   | 1:83:A:ARG:N  | 6        | 3.12          |
| (1,66)  | 1:56:A:GLN:N  | 1:56:A:GLN:CA  | 1:56:A:GLN:C   | 1:57:A:SER:N  | 10       | 3.11          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 3        | 2.96          |
| (1,12)  | 1:28:A:MET:N  | 1:28:A:MET:CA  | 1:28:A:MET:C   | 1:29:A:SER:N  | 16       | 2.95          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 1        | 2.93          |
| (1,112) | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C   | 1:83:A:ARG:N  | 8        | 2.92          |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 8        | 2.9           |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 14       | 2.89          |
| (1,34)  | 1:39:A:ASP:N  | 1:39:A:ASP:CA  | 1:39:A:ASP:C   | 1:40:A:ILE:N  | 15       | 2.87          |
| (1,134) | 1:93:A:LEU:N  | 1:93:A:LEU:CA  | 1:93:A:LEU:C   | 1:94:A:GLN:N  | 15       | 2.77          |
| (1,165) | 2:221:B:GLU:C | 2:222:B:ALA:N  | 2:222:B:ALA:CA | 2:222:B:ALA:C | 13       | 2.76          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 3        | 2.76          |
| (1,65)  | 1:55:A:ILE:C  | 1:56:A:GLN:N   | 1:56:A:GLN:CA  | 1:56:A:GLN:C  | 16       | 2.74          |
| (1,134) | 1:93:A:LEU:N  | 1:93:A:LEU:CA  | 1:93:A:LEU:C   | 1:94:A:GLN:N  | 13       | 2.71          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 19       | 2.69          |
| (1,140) | 2:206:B:ARG:N | 2:206:B:ARG:CA | 2:206:B:ARG:C  | 2:207:B:VAL:N | 20       | 2.68          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 8        | 2.68          |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 1        | 2.65          |
| (1,66)  | 1:56:A:GLN:N  | 1:56:A:GLN:CA  | 1:56:A:GLN:C   | 1:57:A:SER:N  | 2        | 2.64          |
| (1,62)  | 1:54:A:ILE:N  | 1:54:A:ILE:CA  | 1:54:A:ILE:C   | 1:55:A:ILE:N  | 4        | 2.64          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 2        | 2.62          |
| (1,12)  | 1:28:A:MET:N  | 1:28:A:MET:CA  | 1:28:A:MET:C   | 1:29:A:SER:N  | 14       | 2.62          |
| (1,137) | 2:204:B:THR:C | 2:205:B:TRP:N  | 2:205:B:TRP:CA | 2:205:B:TRP:C | 3        | 2.57          |
| (1,112) | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C   | 1:83:A:ARG:N  | 15       | 2.56          |
| (1,161) | 2:219:B:THR:C | 2:220:B:ARG:N  | 2:220:B:ARG:CA | 2:220:B:ARG:C | 16       | 2.54          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 18       | 2.54          |
| (1,152) | 2:215:B:LYS:N | 2:215:B:LYS:CA | 2:215:B:LYS:C  | 2:216:B:ILE:N | 3        | 2.5           |
| (1,62)  | 1:54:A:ILE:N  | 1:54:A:ILE:CA  | 1:54:A:ILE:C   | 1:55:A:ILE:N  | 12       | 2.47          |
| (1,64)  | 1:55:A:ILE:N  | 1:55:A:ILE:CA  | 1:55:A:ILE:C   | 1:56:A:GLN:N  | 17       | 2.45          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 6        | 2.44          |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 10       | 2.42          |
| (1,62)  | 1:54:A:ILE:N  | 1:54:A:ILE:CA  | 1:54:A:ILE:C   | 1:55:A:ILE:N  | 14       | 2.41          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 20       | 2.39          |
| (1,112) | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C   | 1:83:A:ARG:N  | 17       | 2.37          |
| (1,82)  | 1:65:A:SER:N  | 1:65:A:SER:CA  | 1:65:A:SER:C   | 1:66:A:ASN:N  | 20       | 2.36          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 10       | 2.35          |
| (1,82)  | 1:65:A:SER:N  | 1:65:A:SER:CA  | 1:65:A:SER:C   | 1:66:A:ASN:N  | 10       | 2.33          |
| (1,75)  | 1:61:A:SER:C  | 1:62:A:LEU:N   | 1:62:A:LEU:CA  | 1:62:A:LEU:C  | 17       | 2.33          |
| (1,158) | 2:218:B:LEU:N | 2:218:B:LEU:CA | 2:218:B:LEU:C  | 2:219:B:THR:N | 8        | 2.32          |
| (1,53)  | 1:49:A:GLY:C  | 1:50:A:ARG:N   | 1:50:A:ARG:CA  | 1:50:A:ARG:C  | 16       | 2.32          |
| (1,135) | 2:203:B:LEU:C | 2:204:B:THR:N  | 2:204:B:THR:CA | 2:204:B:THR:C | 20       | 2.31          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 11       | 2.31          |
| (1,53)  | 1:49:A:GLY:C  | 1:50:A:ARG:N   | 1:50:A:ARG:CA  | 1:50:A:ARG:C  | 4        | 2.29          |
| (1,134) | 1:93:A:LEU:N  | 1:93:A:LEU:CA  | 1:93:A:LEU:C   | 1:94:A:GLN:N  | 9        | 2.28          |
| (1,138) | 2:205:B:TRP:N | 2:205:B:TRP:CA | 2:205:B:TRP:C  | 2:206:B:ARG:N | 6        | 2.26          |
| (1,159) | 2:218:B:LEU:C | 2:219:B:THR:N  | 2:219:B:THR:CA | 2:219:B:THR:C | 10       | 2.25          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 7        | 2.24          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 12       | 2.23          |
| (1,92)  | 1:71:A:GLU:N  | 1:71:A:GLU:CA  | 1:71:A:GLU:C   | 1:72:A:ILE:N  | 7        | 2.23          |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,92)  | 1:71:A:GLU:N  | 1:71:A:GLU:CA  | 1:71:A:GLU:C   | 1:72:A:ILE:N  | 18       | 2.22          |
| (1,84)  | 1:66:A:ASN:N  | 1:66:A:ASN:CA  | 1:66:A:ASN:C   | 1:67:A:PRO:N  | 8        | 2.22          |
| (1,134) | 1:93:A:LEU:N  | 1:93:A:LEU:CA  | 1:93:A:LEU:C   | 1:94:A:GLN:N  | 17       | 2.2           |
| (1,66)  | 1:56:A:GLN:N  | 1:56:A:GLN:CA  | 1:56:A:GLN:C   | 1:57:A:SER:N  | 5        | 2.19          |
| (1,61)  | 1:53:A:HIS:C  | 1:54:A:ILE:N   | 1:54:A:ILE:CA  | 1:54:A:ILE:C  | 11       | 2.15          |
| (1,148) | 2:210:B:SER:N | 2:210:B:SER:CA | 2:210:B:SER:C  | 2:211:B:GLN:N | 8        | 2.13          |
| (1,35)  | 1:39:A:ASP:C  | 1:40:A:ILE:N   | 1:40:A:ILE:CA  | 1:40:A:ILE:C  | 19       | 2.13          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 9        | 2.07          |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 3        | 2.07          |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 6        | 2.06          |
| (1,85)  | 1:67:A:PRO:C  | 1:68:A:ASP:N   | 1:68:A:ASP:CA  | 1:68:A:ASP:C  | 5        | 2.06          |
| (1,164) | 2:221:B:GLU:N | 2:221:B:GLU:CA | 2:221:B:GLU:C  | 2:222:B:ALA:N | 11       | 2.05          |
| (1,145) | 2:208:B:GLN:C | 2:209:B:ARG:N  | 2:209:B:ARG:CA | 2:209:B:ARG:C | 5        | 2.04          |
| (1,58)  | 1:52:A:VAL:N  | 1:52:A:VAL:CA  | 1:52:A:VAL:C   | 1:53:A:HIS:N  | 13       | 2.02          |
| (1,2)   | 1:18:A:ASP:N  | 1:18:A:ASP:CA  | 1:18:A:ASP:C   | 1:19:A:SER:N  | 6        | 2.01          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 15       | 2.0           |
| (1,82)  | 1:65:A:SER:N  | 1:65:A:SER:CA  | 1:65:A:SER:C   | 1:66:A:ASN:N  | 18       | 2.0           |
| (1,166) | 2:222:B:ALA:N | 2:222:B:ALA:CA | 2:222:B:ALA:C  | 2:223:B:PRO:N | 16       | 1.99          |
| (1,92)  | 1:71:A:GLU:N  | 1:71:A:GLU:CA  | 1:71:A:GLU:C   | 1:72:A:ILE:N  | 3        | 1.96          |
| (1,82)  | 1:65:A:SER:N  | 1:65:A:SER:CA  | 1:65:A:SER:C   | 1:66:A:ASN:N  | 1        | 1.94          |
| (1,46)  | 1:46:A:GLU:N  | 1:46:A:GLU:CA  | 1:46:A:GLU:C   | 1:47:A:LYS:N  | 1        | 1.94          |
| (1,153) | 2:215:B:LYS:C | 2:216:B:ILE:N  | 2:216:B:ILE:CA | 2:216:B:ILE:C | 18       | 1.85          |
| (1,134) | 1:93:A:LEU:N  | 1:93:A:LEU:CA  | 1:93:A:LEU:C   | 1:94:A:GLN:N  | 8        | 1.83          |
| (1,166) | 2:222:B:ALA:N | 2:222:B:ALA:CA | 2:222:B:ALA:C  | 2:223:B:PRO:N | 11       | 1.82          |
| (1,74)  | 1:61:A:SER:N  | 1:61:A:SER:CA  | 1:61:A:SER:C   | 1:62:A:LEU:N  | 10       | 1.79          |
| (1,35)  | 1:39:A:ASP:C  | 1:40:A:ILE:N   | 1:40:A:ILE:CA  | 1:40:A:ILE:C  | 1        | 1.79          |
| (1,130) | 1:91:A:SER:N  | 1:91:A:SER:CA  | 1:91:A:SER:C   | 1:92:A:CYS:N  | 17       | 1.78          |
| (1,83)  | 1:65:A:SER:C  | 1:66:A:ASN:N   | 1:66:A:ASN:CA  | 1:66:A:ASN:C  | 17       | 1.76          |
| (1,92)  | 1:71:A:GLU:N  | 1:71:A:GLU:CA  | 1:71:A:GLU:C   | 1:72:A:ILE:N  | 6        | 1.75          |
| (1,31)  | 1:37:A:SER:C  | 1:38:A:LEU:N   | 1:38:A:LEU:CA  | 1:38:A:LEU:C  | 2        | 1.74          |
| (1,83)  | 1:65:A:SER:C  | 1:66:A:ASN:N   | 1:66:A:ASN:CA  | 1:66:A:ASN:C  | 15       | 1.73          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 9        | 1.7           |
| (1,66)  | 1:56:A:GLN:N  | 1:56:A:GLN:CA  | 1:56:A:GLN:C   | 1:57:A:SER:N  | 6        | 1.7           |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 20       | 1.66          |
| (1,46)  | 1:46:A:GLU:N  | 1:46:A:GLU:CA  | 1:46:A:GLU:C   | 1:47:A:LYS:N  | 4        | 1.64          |
| (1,31)  | 1:37:A:SER:C  | 1:38:A:LEU:N   | 1:38:A:LEU:CA  | 1:38:A:LEU:C  | 5        | 1.64          |
| (1,92)  | 1:71:A:GLU:N  | 1:71:A:GLU:CA  | 1:71:A:GLU:C   | 1:72:A:ILE:N  | 11       | 1.63          |
| (1,46)  | 1:46:A:GLU:N  | 1:46:A:GLU:CA  | 1:46:A:GLU:C   | 1:47:A:LYS:N  | 16       | 1.62          |
| (1,134) | 1:93:A:LEU:N  | 1:93:A:LEU:CA  | 1:93:A:LEU:C   | 1:94:A:GLN:N  | 18       | 1.58          |
| (1,120) | 1:86:A:GLU:N  | 1:86:A:GLU:CA  | 1:86:A:GLU:C   | 1:87:A:ARG:N  | 4        | 1.55          |
| (1,62)  | 1:54:A:ILE:N  | 1:54:A:ILE:CA  | 1:54:A:ILE:C   | 1:55:A:ILE:N  | 5        | 1.55          |
| (1,12)  | 1:28:A:MET:N  | 1:28:A:MET:CA  | 1:28:A:MET:C   | 1:29:A:SER:N  | 6        | 1.55          |
| (1,153) | 2:215:B:LYS:C | 2:216:B:ILE:N  | 2:216:B:ILE:CA | 2:216:B:ILE:C | 5        | 1.54          |
| (1,20)  | 1:32:A:GLU:N  | 1:32:A:GLU:CA  | 1:32:A:GLU:C   | 1:33:A:LYS:N  | 20       | 1.53          |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 7        | 1.48          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 1        | 1.46          |
| (1,112) | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C   | 1:83:A:ARG:N  | 9        | 1.44          |
| (1,83)  | 1:65:A:SER:C  | 1:66:A:ASN:N   | 1:66:A:ASN:CA  | 1:66:A:ASN:C  | 20       | 1.44          |
| (1,46)  | 1:46:A:GLU:N  | 1:46:A:GLU:CA  | 1:46:A:GLU:C   | 1:47:A:LYS:N  | 17       | 1.44          |
| (1,35)  | 1:39:A:ASP:C  | 1:40:A:ILE:N   | 1:40:A:ILE:CA  | 1:40:A:ILE:C  | 8        | 1.44          |
| (1,31)  | 1:37:A:SER:C  | 1:38:A:LEU:N   | 1:38:A:LEU:CA  | 1:38:A:LEU:C  | 15       | 1.44          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,35)  | 1:39:A:ASP:C  | 1:40:A:ILE:N   | 1:40:A:ILE:CA  | 1:40:A:ILE:C  | 12       | 1.43          |
| (1,12)  | 1:28:A:MET:N  | 1:28:A:MET:CA  | 1:28:A:MET:C   | 1:29:A:SER:N  | 9        | 1.42          |
| (1,65)  | 1:55:A:ILE:C  | 1:56:A:GLN:N   | 1:56:A:GLN:CA  | 1:56:A:GLN:C  | 13       | 1.38          |
| (1,22)  | 1:33:A:LYS:N  | 1:33:A:LYS:CA  | 1:33:A:LYS:C   | 1:34:A:ARG:N  | 15       | 1.37          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 15       | 1.36          |
| (1,12)  | 1:28:A:MET:N  | 1:28:A:MET:CA  | 1:28:A:MET:C   | 1:29:A:SER:N  | 10       | 1.35          |
| (1,35)  | 1:39:A:ASP:C  | 1:40:A:ILE:N   | 1:40:A:ILE:CA  | 1:40:A:ILE:C  | 7        | 1.33          |
| (1,35)  | 1:39:A:ASP:C  | 1:40:A:ILE:N   | 1:40:A:ILE:CA  | 1:40:A:ILE:C  | 9        | 1.32          |
| (1,135) | 2:203:B:LEU:C | 2:204:B:THR:N  | 2:204:B:THR:CA | 2:204:B:THR:C | 19       | 1.31          |
| (1,140) | 2:206:B:ARG:N | 2:206:B:ARG:CA | 2:206:B:ARG:C  | 2:207:B:VAL:N | 8        | 1.29          |
| (1,2)   | 1:18:A:ASP:N  | 1:18:A:ASP:CA  | 1:18:A:ASP:C   | 1:19:A:SER:N  | 17       | 1.29          |
| (1,135) | 2:203:B:LEU:C | 2:204:B:THR:N  | 2:204:B:THR:CA | 2:204:B:THR:C | 5        | 1.28          |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 12       | 1.28          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 11       | 1.27          |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 13       | 1.27          |
| (1,64)  | 1:55:A:ILE:N  | 1:55:A:ILE:CA  | 1:55:A:ILE:C   | 1:56:A:GLN:N  | 8        | 1.27          |
| (1,63)  | 1:54:A:ILE:C  | 1:55:A:ILE:N   | 1:55:A:ILE:CA  | 1:55:A:ILE:C  | 4        | 1.27          |
| (1,88)  | 1:69:A:GLU:N  | 1:69:A:GLU:CA  | 1:69:A:GLU:C   | 1:70:A:ILE:N  | 18       | 1.26          |
| (1,68)  | 1:57:A:SER:N  | 1:57:A:SER:CA  | 1:57:A:SER:C   | 1:58:A:ARG:N  | 12       | 1.26          |
| (1,149) | 2:211:B:GLN:C | 2:212:B:ASN:N  | 2:212:B:ASN:CA | 2:212:B:ASN:C | 16       | 1.25          |
| (1,12)  | 1:28:A:MET:N  | 1:28:A:MET:CA  | 1:28:A:MET:C   | 1:29:A:SER:N  | 12       | 1.23          |
| (1,53)  | 1:49:A:GLY:C  | 1:50:A:ARG:N   | 1:50:A:ARG:CA  | 1:50:A:ARG:C  | 8        | 1.22          |
| (1,53)  | 1:49:A:GLY:C  | 1:50:A:ARG:N   | 1:50:A:ARG:CA  | 1:50:A:ARG:C  | 3        | 1.19          |
| (1,134) | 1:93:A:LEU:N  | 1:93:A:LEU:CA  | 1:93:A:LEU:C   | 1:94:A:GLN:N  | 4        | 1.18          |
| (1,30)  | 1:37:A:SER:N  | 1:37:A:SER:CA  | 1:37:A:SER:C   | 1:38:A:LEU:N  | 1        | 1.18          |
| (1,146) | 2:209:B:ARG:N | 2:209:B:ARG:CA | 2:209:B:ARG:C  | 2:210:B:SER:N | 14       | 1.17          |
| (1,90)  | 1:70:A:ILE:N  | 1:70:A:ILE:CA  | 1:70:A:ILE:C   | 1:71:A:GLU:N  | 16       | 1.17          |
| (1,124) | 1:88:A:TYR:N  | 1:88:A:TYR:CA  | 1:88:A:TYR:C   | 1:89:A:VAL:N  | 10       | 1.15          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 8        | 1.15          |
| (1,94)  | 1:72:A:ILE:N  | 1:72:A:ILE:CA  | 1:72:A:ILE:C   | 1:73:A:ASP:N  | 16       | 1.15          |
| (1,92)  | 1:71:A:GLU:N  | 1:71:A:GLU:CA  | 1:71:A:GLU:C   | 1:72:A:ILE:N  | 16       | 1.15          |
| (1,5)   | 1:21:A:GLU:C  | 1:22:A:GLU:N   | 1:22:A:GLU:CA  | 1:22:A:GLU:C  | 11       | 1.14          |
| (1,96)  | 1:73:A:ASP:N  | 1:73:A:ASP:CA  | 1:73:A:ASP:C   | 1:74:A:PHE:N  | 16       | 1.11          |
| (1,82)  | 1:65:A:SER:N  | 1:65:A:SER:CA  | 1:65:A:SER:C   | 1:66:A:ASN:N  | 2        | 1.1           |
| (1,33)  | 1:38:A:LEU:C  | 1:39:A:ASP:N   | 1:39:A:ASP:CA  | 1:39:A:ASP:C  | 11       | 1.09          |
| (1,112) | 1:82:A:LEU:N  | 1:82:A:LEU:CA  | 1:82:A:LEU:C   | 1:83:A:ARG:N  | 18       | 1.03          |
| (1,58)  | 1:52:A:VAL:N  | 1:52:A:VAL:CA  | 1:52:A:VAL:C   | 1:53:A:HIS:N  | 9        | 1.03          |
| (1,3)   | 1:18:A:ASP:C  | 1:19:A:SER:N   | 1:19:A:SER:CA  | 1:19:A:SER:C  | 11       | 1.03          |