



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:26 PM UTC

PDB ID : 2LGD / pdb\_00002lgd  
BMRB ID : 17805  
Title : The high resolution structure of ubiquitin like domain of UBLCP1  
Authors : Lee, W.; Ko, S.  
Deposited on : 2011-07-25

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

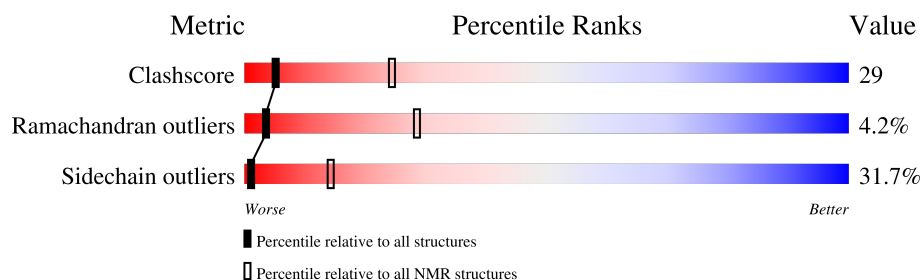
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

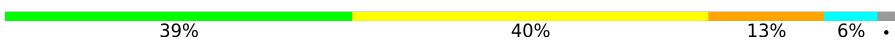
The overall completeness of chemical shifts assignment is 88%.

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     | 83     |  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:2-A:77 (76)         | 0.19              | 1            |

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

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

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

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1306 atoms, of which 679 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin-like domain-containing CTD phosphatase 1.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 81       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1306  | 402 | 679 | 104 | 117 | 4 |       |

There are 2 discrepancies between the modelled and reference sequences:

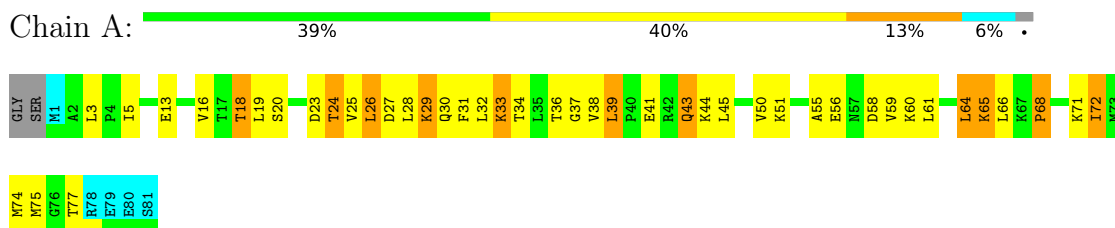
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -1      | GLY      | -      | expression tag | UNP Q8WVY7 |
| A     | 0       | SER      | -      | expression tag | UNP Q8WVY7 |

## 4 Residue-property plots

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

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

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1

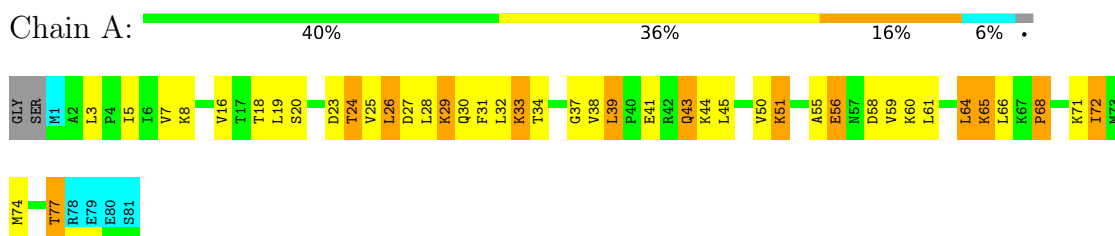


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1 (medoid)

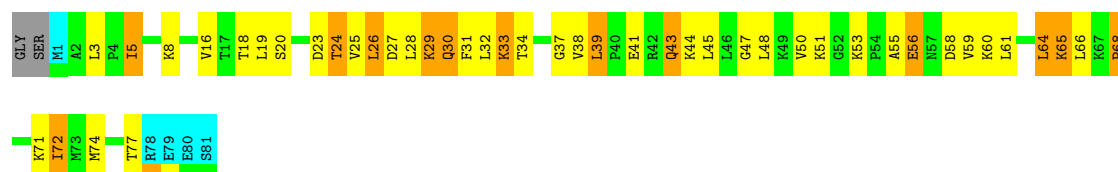
- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1



#### 4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1

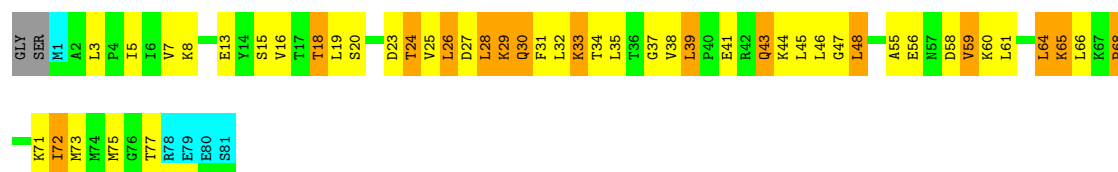




### 4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1

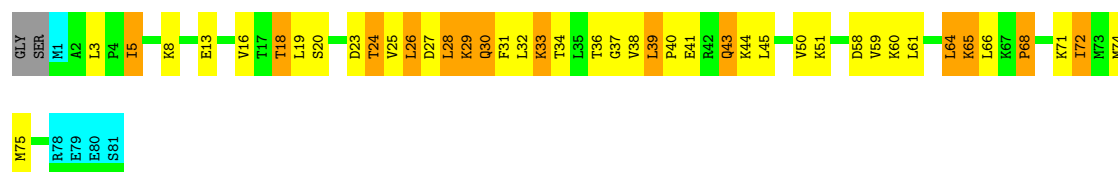
Chain A: 34% 40% 18% 6% .



### 4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1

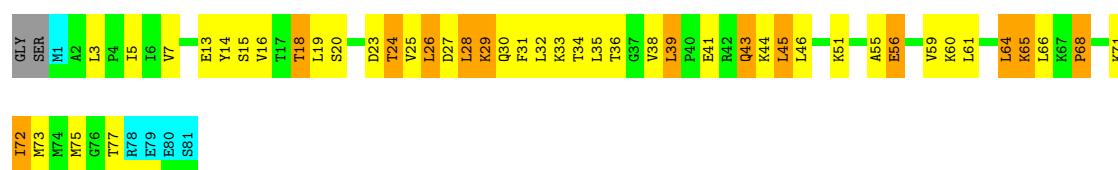
Chain A: 40% 35% 17% 6% .



### 4.2.5 Score per residue for model 5

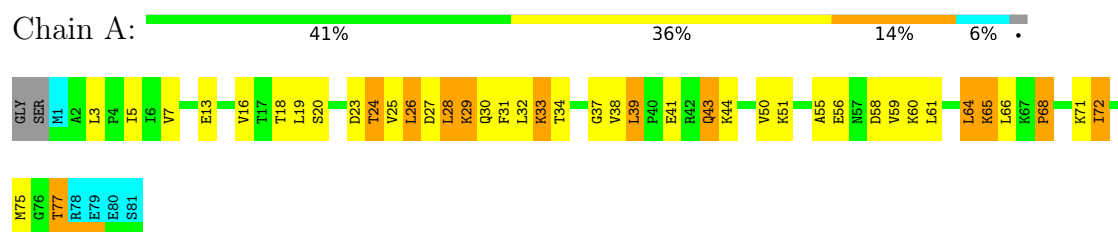
- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1

Chain A: 36% 40% 16% 6% .



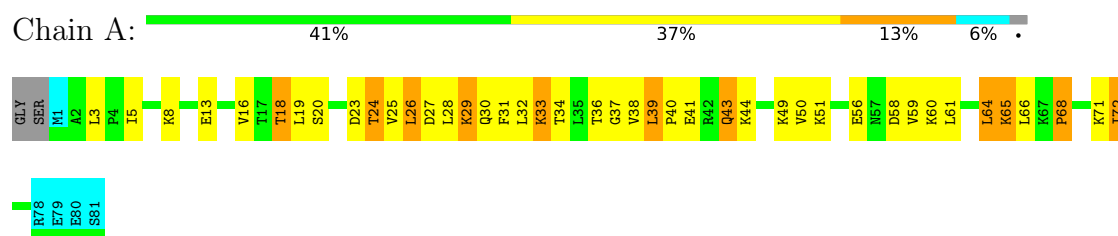
### 4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1



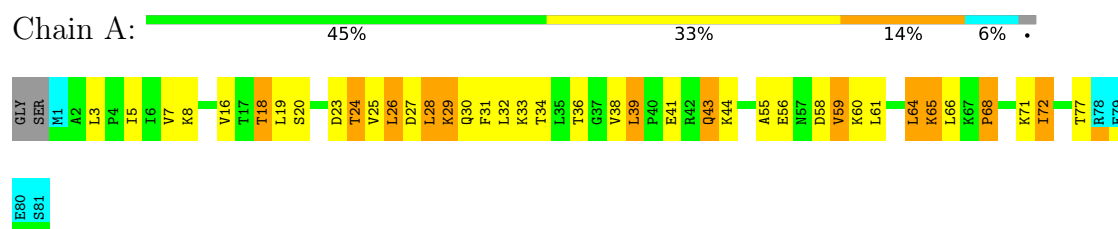
#### 4.2.7 Score per residue for model 7

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1



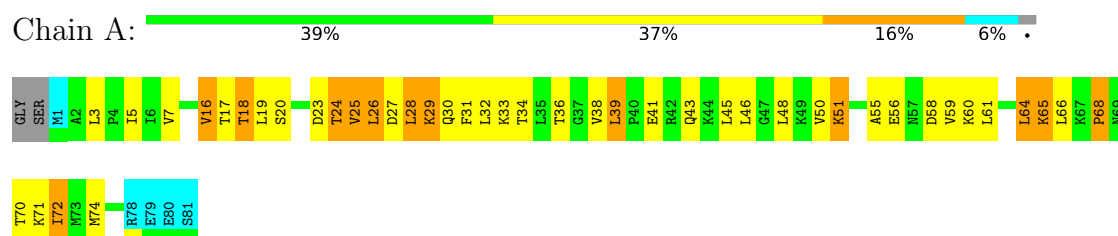
#### 4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1



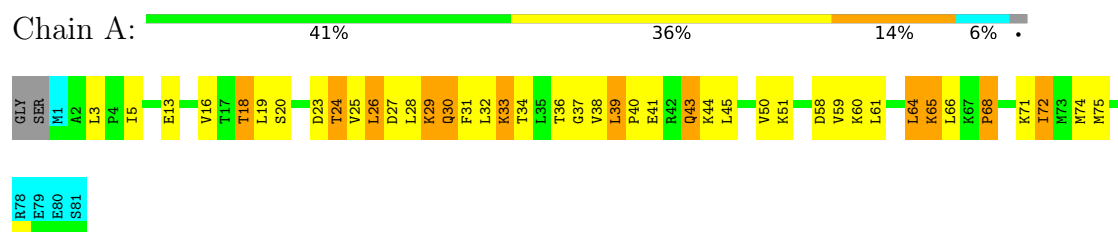
#### 4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1



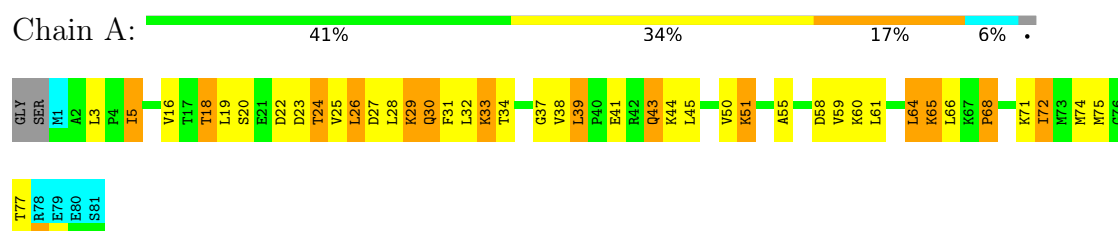
#### 4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1



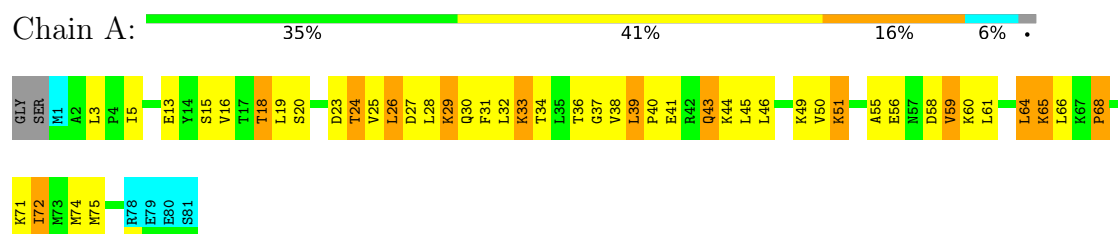
#### 4.2.11 Score per residue for model 11

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1



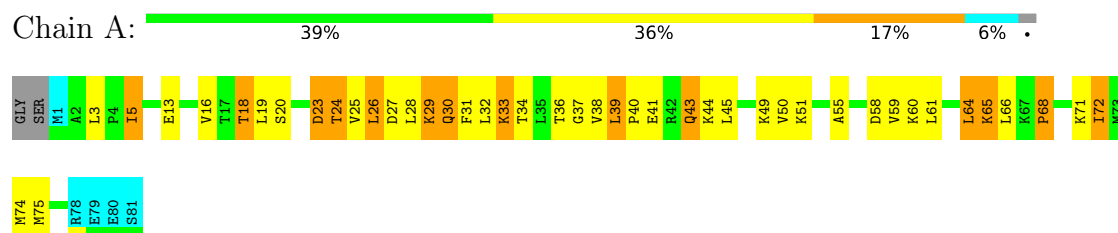
#### 4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1



#### 4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1

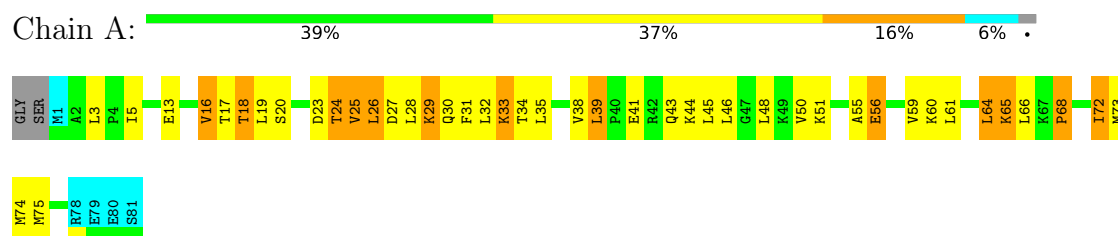






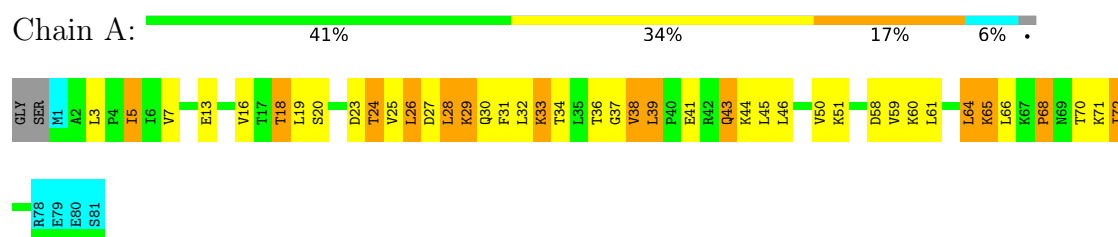
### 4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1



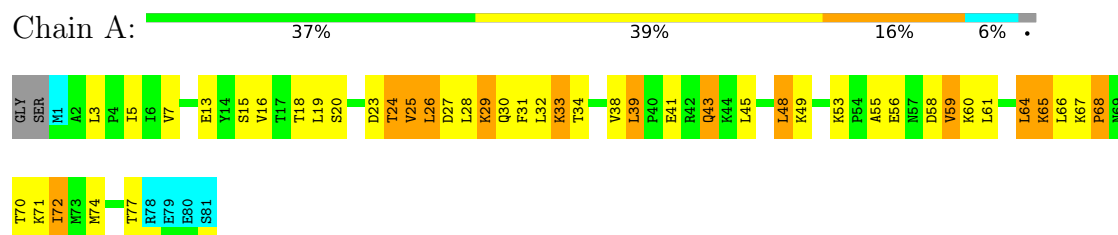
### 4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1



### 4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin-like domain-containing CTD phosphatase 1



## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| PROCHECKNMR   | refinement         |         |
| TALOS         | structure solution |         |
| CYANA         | refinement         | 2.2.5   |
| CYANA         | structure solution | 2.2.5   |

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                       | 971            |
| Number of shifts mapped to atoms             | 971            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 88%            |

## 6 Model quality [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

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     | 584   | 640      | 640      | 35±4    |
| All | All   | 11680 | 12800    | 12800    | 705     |

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 29.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:7:VAL:HG21  | 1:A:32:LEU:HD22 | 0.97     | 1.36        | 16     | 10    |
| 1:A:18:THR:HG23 | 1:A:19:LEU:HD23 | 0.90     | 1.42        | 8      | 20    |
| 1:A:66:LEU:HD21 | 1:A:72:ILE:HG23 | 0.84     | 1.47        | 3      | 20    |
| 1:A:38:VAL:HG11 | 1:A:43:GLN:CD   | 0.73     | 2.09        | 20     | 7     |
| 1:A:45:LEU:HD23 | 1:A:73:MET:O    | 0.73     | 1.84        | 14     | 5     |
| 1:A:28:LEU:HD23 | 1:A:32:LEU:HD23 | 0.72     | 1.61        | 5      | 7     |
| 1:A:19:LEU:HD13 | 1:A:27:ASP:CG   | 0.69     | 2.11        | 1      | 20    |
| 1:A:7:VAL:CG2   | 1:A:32:LEU:HD22 | 0.67     | 2.18        | 3      | 7     |
| 1:A:45:LEU:HD22 | 1:A:72:ILE:HB   | 0.67     | 1.66        | 17     | 5     |
| 1:A:45:LEU:HD13 | 1:A:72:ILE:HD12 | 0.65     | 1.68        | 18     | 1     |
| 1:A:39:LEU:N    | 1:A:39:LEU:HD13 | 0.65     | 2.05        | 17     | 19    |
| 1:A:29:LYS:HE2  | 1:A:32:LEU:HD21 | 0.65     | 1.66        | 5      | 20    |
| 1:A:19:LEU:HD12 | 1:A:23:ASP:HB2  | 0.63     | 1.70        | 13     | 6     |
| 1:A:43:GLN:OE1  | 1:A:74:MET:HE2  | 0.61     | 1.95        | 16     | 4     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:31:PHE:O    | 1:A:34:THR:HG22 | 0.61     | 1.95        | 8      | 20    |
| 1:A:56:GLU:O    | 1:A:59:VAL:HG12 | 0.61     | 1.95        | 3      | 4     |
| 1:A:18:THR:HG21 | 1:A:31:PHE:CD1  | 0.61     | 2.31        | 19     | 13    |
| 1:A:45:LEU:HD23 | 1:A:73:MET:C    | 0.60     | 2.20        | 17     | 4     |
| 1:A:3:LEU:HD12  | 1:A:68:PRO:HG3  | 0.60     | 1.74        | 15     | 9     |
| 1:A:50:VAL:HG22 | 1:A:51:LYS:HG2  | 0.60     | 1.73        | 13     | 12    |
| 1:A:59:VAL:HG11 | 1:A:64:LEU:HD21 | 0.60     | 1.72        | 5      | 16    |
| 1:A:66:LEU:CD2  | 1:A:72:ILE:HG23 | 0.60     | 2.23        | 3      | 18    |
| 1:A:19:LEU:HD13 | 1:A:27:ASP:OD1  | 0.58     | 1.98        | 6      | 14    |
| 1:A:26:LEU:O    | 1:A:26:LEU:HD12 | 0.58     | 1.97        | 18     | 20    |
| 1:A:39:LEU:HD13 | 1:A:39:LEU:H    | 0.57     | 1.57        | 3      | 19    |
| 1:A:47:GLY:O    | 1:A:48:LEU:HD22 | 0.57     | 1.98        | 2      | 2     |
| 1:A:19:LEU:HD12 | 1:A:23:ASP:HB3  | 0.57     | 1.76        | 10     | 14    |
| 1:A:39:LEU:H    | 1:A:39:LEU:HD13 | 0.57     | 1.58        | 12     | 1     |
| 1:A:32:LEU:O    | 1:A:36:THR:HG23 | 0.56     | 2.01        | 13     | 11    |
| 1:A:7:VAL:HG21  | 1:A:32:LEU:CD2  | 0.56     | 2.23        | 16     | 4     |
| 1:A:39:LEU:HD13 | 1:A:39:LEU:N    | 0.56     | 2.16        | 12     | 1     |
| 1:A:46:LEU:HD12 | 1:A:73:MET:HB2  | 0.56     | 1.77        | 3      | 3     |
| 1:A:38:VAL:HG11 | 1:A:43:GLN:NE2  | 0.55     | 2.15        | 9      | 6     |
| 1:A:43:GLN:HE21 | 1:A:74:MET:HE2  | 0.55     | 1.61        | 20     | 1     |
| 1:A:38:VAL:HG21 | 1:A:43:GLN:OE1  | 0.54     | 2.02        | 19     | 6     |
| 1:A:43:GLN:NE2  | 1:A:74:MET:HE2  | 0.54     | 2.18        | 14     | 4     |
| 1:A:50:VAL:HB   | 1:A:64:LEU:HD23 | 0.53     | 1.79        | 15     | 13    |
| 1:A:14:TYR:CD2  | 1:A:36:THR:HG22 | 0.53     | 2.38        | 16     | 2     |
| 1:A:38:VAL:HG13 | 1:A:77:THR:O    | 0.53     | 2.03        | 6      | 8     |
| 1:A:29:LYS:CE   | 1:A:32:LEU:HD21 | 0.53     | 2.32        | 5      | 6     |
| 1:A:45:LEU:HD12 | 1:A:72:ILE:HB   | 0.52     | 1.81        | 9      | 6     |
| 1:A:48:LEU:O    | 1:A:64:LEU:HD22 | 0.52     | 2.03        | 9      | 3     |
| 1:A:43:GLN:NE2  | 1:A:77:THR:H    | 0.52     | 2.03        | 11     | 1     |
| 1:A:18:THR:HG23 | 1:A:19:LEU:CD2  | 0.52     | 2.29        | 3      | 5     |
| 1:A:45:LEU:HD21 | 1:A:74:MET:HG3  | 0.52     | 1.81        | 18     | 3     |
| 1:A:39:LEU:H    | 1:A:39:LEU:HD22 | 0.51     | 1.65        | 18     | 20    |
| 1:A:14:TYR:CE2  | 1:A:36:THR:HG22 | 0.51     | 2.40        | 16     | 1     |
| 1:A:5:ILE:HB    | 1:A:28:LEU:HD11 | 0.51     | 1.83        | 19     | 4     |
| 1:A:29:LYS:CE   | 1:A:45:LEU:HD13 | 0.50     | 2.36        | 5      | 1     |
| 1:A:34:THR:HG23 | 1:A:35:LEU:HD23 | 0.50     | 1.82        | 16     | 4     |
| 1:A:39:LEU:HD23 | 1:A:41:GLU:CG   | 0.49     | 2.37        | 1      | 20    |
| 1:A:29:LYS:NZ   | 1:A:45:LEU:HD13 | 0.49     | 2.22        | 5      | 1     |
| 1:A:23:ASP:O    | 1:A:24:THR:HG23 | 0.49     | 2.08        | 3      | 20    |
| 1:A:33:LYS:NZ   | 1:A:39:LEU:HD12 | 0.49     | 2.22        | 1      | 3     |
| 1:A:39:LEU:N    | 1:A:39:LEU:CD1  | 0.49     | 2.76        | 17     | 12    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:5:ILE:CG2   | 1:A:72:ILE:HD11 | 0.48     | 2.39        | 11     | 2     |
| 1:A:3:LEU:HD12  | 1:A:68:PRO:CG   | 0.48     | 2.37        | 6      | 9     |
| 1:A:28:LEU:CD2  | 1:A:32:LEU:HD23 | 0.48     | 2.39        | 9      | 4     |
| 1:A:7:VAL:HG13  | 1:A:45:LEU:HD21 | 0.47     | 1.84        | 5      | 3     |
| 1:A:64:LEU:HD12 | 1:A:65:LYS:H    | 0.47     | 1.69        | 8      | 20    |
| 1:A:38:VAL:HG21 | 1:A:43:GLN:NE2  | 0.47     | 2.25        | 16     | 3     |
| 1:A:19:LEU:HD12 | 1:A:23:ASP:CB   | 0.47     | 2.39        | 16     | 5     |
| 1:A:38:VAL:HG21 | 1:A:43:GLN:CD   | 0.46     | 2.35        | 16     | 7     |
| 1:A:61:LEU:O    | 1:A:65:LYS:HB2  | 0.46     | 2.11        | 2      | 20    |
| 1:A:19:LEU:HD21 | 1:A:28:LEU:HA   | 0.46     | 1.87        | 9      | 1     |
| 1:A:18:THR:HG21 | 1:A:31:PHE:CE1  | 0.46     | 2.45        | 19     | 1     |
| 1:A:66:LEU:HD22 | 1:A:70:THR:CG2  | 0.46     | 2.41        | 19     | 4     |
| 1:A:32:LEU:HD12 | 1:A:33:LYS:N    | 0.46     | 2.25        | 13     | 5     |
| 1:A:33:LYS:O    | 1:A:37:GLY:N    | 0.45     | 2.48        | 10     | 15    |
| 1:A:24:THR:HG22 | 1:A:58:ASP:O    | 0.45     | 2.12        | 3      | 17    |
| 1:A:3:LEU:HD22  | 1:A:68:PRO:CG   | 0.45     | 2.42        | 12     | 11    |
| 1:A:40:PRO:O    | 1:A:43:GLN:O    | 0.45     | 2.35        | 12     | 6     |
| 1:A:39:LEU:N    | 1:A:39:LEU:HD22 | 0.44     | 2.27        | 18     | 2     |
| 1:A:38:VAL:HG11 | 1:A:43:GLN:OE1  | 0.44     | 2.11        | 3      | 3     |
| 1:A:43:GLN:HB3  | 1:A:75:MET:O    | 0.44     | 2.11        | 11     | 1     |
| 1:A:45:LEU:HD11 | 1:A:74:MET:HG3  | 0.44     | 1.89        | 4      | 9     |
| 1:A:19:LEU:HD22 | 1:A:27:ASP:OD1  | 0.44     | 2.12        | 9      | 1     |
| 1:A:59:VAL:CG1  | 1:A:64:LEU:HD11 | 0.44     | 2.42        | 15     | 1     |
| 1:A:39:LEU:HD23 | 1:A:41:GLU:HG3  | 0.44     | 1.89        | 14     | 10    |
| 1:A:5:ILE:HG21  | 1:A:72:ILE:HD11 | 0.44     | 1.90        | 11     | 2     |
| 1:A:3:LEU:HD22  | 1:A:68:PRO:CB   | 0.44     | 2.43        | 17     | 11    |
| 1:A:50:VAL:HG22 | 1:A:51:LYS:HG3  | 0.44     | 1.89        | 6      | 1     |
| 1:A:43:GLN:HB2  | 1:A:75:MET:O    | 0.43     | 2.13        | 16     | 3     |
| 1:A:45:LEU:O    | 1:A:46:LEU:C    | 0.42     | 2.63        | 3      | 1     |
| 1:A:26:LEU:O    | 1:A:30:GLN:HB3  | 0.42     | 2.14        | 18     | 2     |
| 1:A:3:LEU:HD22  | 1:A:68:PRO:HG3  | 0.42     | 1.91        | 14     | 5     |
| 1:A:16:VAL:O    | 1:A:17:THR:HG23 | 0.42     | 2.14        | 9      | 2     |
| 1:A:27:ASP:O    | 1:A:30:GLN:HG3  | 0.41     | 2.14        | 8      | 16    |
| 1:A:25:VAL:HG12 | 1:A:26:LEU:N    | 0.41     | 2.30        | 18     | 3     |
| 1:A:33:LYS:HB2  | 1:A:38:VAL:O    | 0.41     | 2.15        | 15     | 4     |
| 1:A:59:VAL:HG21 | 1:A:64:LEU:HD21 | 0.41     | 1.90        | 20     | 2     |
| 1:A:46:LEU:HD13 | 1:A:73:MET:CB   | 0.41     | 2.45        | 5      | 1     |
| 1:A:38:VAL:CG1  | 1:A:43:GLN:CD   | 0.41     | 2.90        | 20     | 1     |
| 1:A:39:LEU:HD23 | 1:A:41:GLU:HG2  | 0.41     | 1.93        | 18     | 2     |
| 1:A:28:LEU:HD13 | 1:A:61:LEU:HG   | 0.40     | 1.92        | 6      | 1     |
| 1:A:50:VAL:HG22 | 1:A:51:LYS:CG   | 0.40     | 2.46        | 6      | 1     |

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| Atom-1         | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|----------------|----------------|----------|-------------|--------|-------|
|                |                |          |             | Worst  | Total |
| 1:A:39:LEU:CD2 | 1:A:42:ARG:HB2 | 0.40     | 2.46        | 17     | 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     | 76/83 (92%)     | 64±1 (84±1%) | 9±1 (12±2%) | 3±1 (4±1%) | 3           | 28 |
| All | All   | 1520/1660 (92%) | 1278 (84%)   | 178 (12%)   | 64 (4%)    | 3           | 28 |

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 65  | LYS  | 20             |
| 1   | A     | 68  | PRO  | 20             |
| 1   | A     | 55  | ALA  | 16             |
| 1   | A     | 56  | GLU  | 6              |
| 1   | A     | 47  | GLY  | 2              |

### 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     | 66/72 (92%)     | 45±2 (68±3%) | 21±2 (32±3%) | 1           | 14 |
| All | All   | 1320/1440 (92%) | 901 (68%)    | 419 (32%)    | 1           | 14 |

All 37 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     | 5   | ILE  | 20             |
| 1   | A     | 16  | VAL  | 20             |
| 1   | A     | 20  | SER  | 20             |
| 1   | A     | 24  | THR  | 20             |
| 1   | A     | 25  | VAL  | 20             |
| 1   | A     | 26  | LEU  | 20             |
| 1   | A     | 29  | LYS  | 20             |
| 1   | A     | 33  | LYS  | 20             |
| 1   | A     | 39  | LEU  | 20             |
| 1   | A     | 60  | LYS  | 20             |
| 1   | A     | 64  | LEU  | 20             |
| 1   | A     | 72  | ILE  | 20             |
| 1   | A     | 28  | LEU  | 18             |
| 1   | A     | 43  | GLN  | 18             |
| 1   | A     | 71  | LYS  | 18             |
| 1   | A     | 44  | LYS  | 17             |
| 1   | A     | 13  | GLU  | 15             |
| 1   | A     | 18  | THR  | 15             |
| 1   | A     | 8   | LYS  | 9              |
| 1   | A     | 30  | GLN  | 9              |
| 1   | A     | 75  | MET  | 9              |
| 1   | A     | 56  | GLU  | 8              |
| 1   | A     | 51  | LYS  | 6              |
| 1   | A     | 77  | THR  | 4              |
| 1   | A     | 15  | SER  | 4              |
| 1   | A     | 59  | VAL  | 4              |
| 1   | A     | 45  | LEU  | 4              |
| 1   | A     | 49  | LYS  | 4              |
| 1   | A     | 46  | LEU  | 4              |
| 1   | A     | 53  | LYS  | 3              |
| 1   | A     | 48  | LEU  | 3              |
| 1   | A     | 38  | VAL  | 2              |
| 1   | A     | 22  | ASP  | 1              |
| 1   | A     | 23  | ASP  | 1              |
| 1   | A     | 65  | LYS  | 1              |
| 1   | A     | 74  | MET  | 1              |
| 1   | A     | 67  | LYS  | 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 88% for the well-defined parts and 86% 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                  | 971 |
| Number of shifts mapped to atoms        | 971 |
| 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           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 80       | $-0.69 \pm 0.19$                | Should be checked          |
| $^{13}\text{C}_\beta$  | 73       | $-0.01 \pm 0.15$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 71       | $-1.28 \pm 0.49$                | Should be applied          |
| $^{15}\text{N}$        | 76       | $0.31 \pm 0.29$                 | 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 88%, i.e. 934 atoms were assigned a chemical shift out of a possible 1062. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 371/379 (98%) | 155/155 (100%) | 144/152 (95%)   | 72/72 (100%)    |
| Sidechain | 555/652 (85%) | 383/427 (90%)  | 172/206 (83%)   | 0/19 (0%)       |

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|          | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 8/31 (26%)     | 7/15 (47%)     | 0/15 (0%)       | 1/1 (100%)      |
| Overall  | 934/1062 (88%) | 545/597 (91%)  | 316/373 (85%)   | 73/92 (79%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 971 atoms were assigned a chemical shift out of a possible 1132. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 390/404 (97%)  | 163/165 (99%)  | 151/162 (93%)   | 76/77 (99%)     |
| Sidechain | 573/697 (82%)  | 395/455 (87%)  | 178/220 (81%)   | 0/22 (0%)       |
| Aromatic  | 8/31 (26%)     | 7/15 (47%)     | 0/15 (0%)       | 1/1 (100%)      |
| Overall   | 971/1132 (86%) | 565/635 (89%)  | 329/397 (83%)   | 77/100 (77%)    |

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

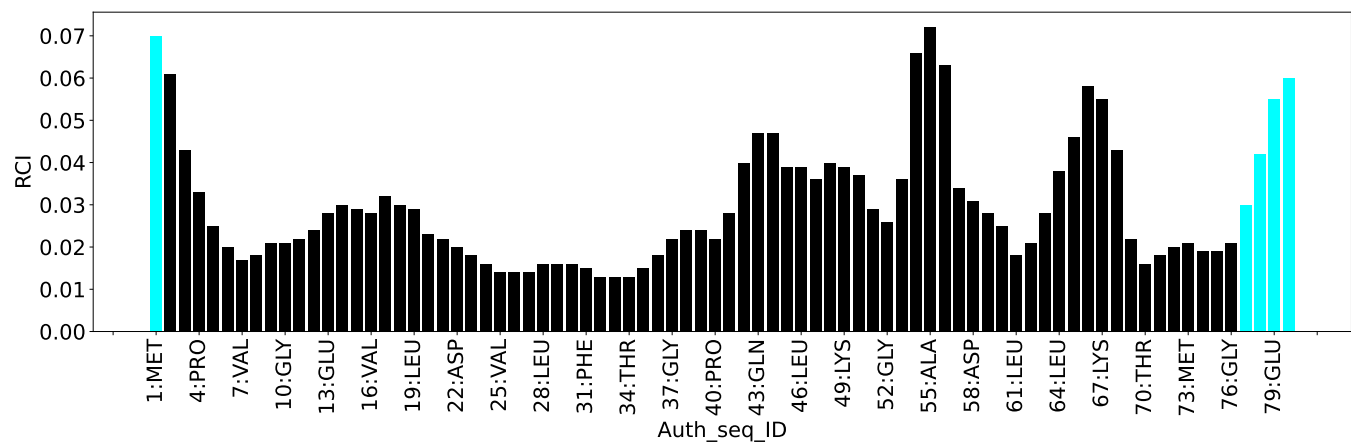
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 36  | THR  | HB   | 2.44       | 2.57 – 5.77         | -5.4    |

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 1914  |
| Intra-residue ( $ i-j =0$ )                              | 403   |
| Sequential ( $ i-j =1$ )                                 | 498   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 339   |
| Long range ( $ i-j \geq 5$ )                             | 646   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 28    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 100   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 24.3  |
| Number of long range restraints per residue <sup>1</sup> | 7.9   |

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

### 8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

#### 8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 18.2                                   | 0.2     |
| 0.2-0.5 (Medium) | 10.8                                   | 0.47    |
| >0.5 (Large)     | 19.6                                   | 3.71    |

### 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)   | 32.7                                   | 10.0    |
| 10.0-20.0 (Medium) | 0.1                                    | 10.86   |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

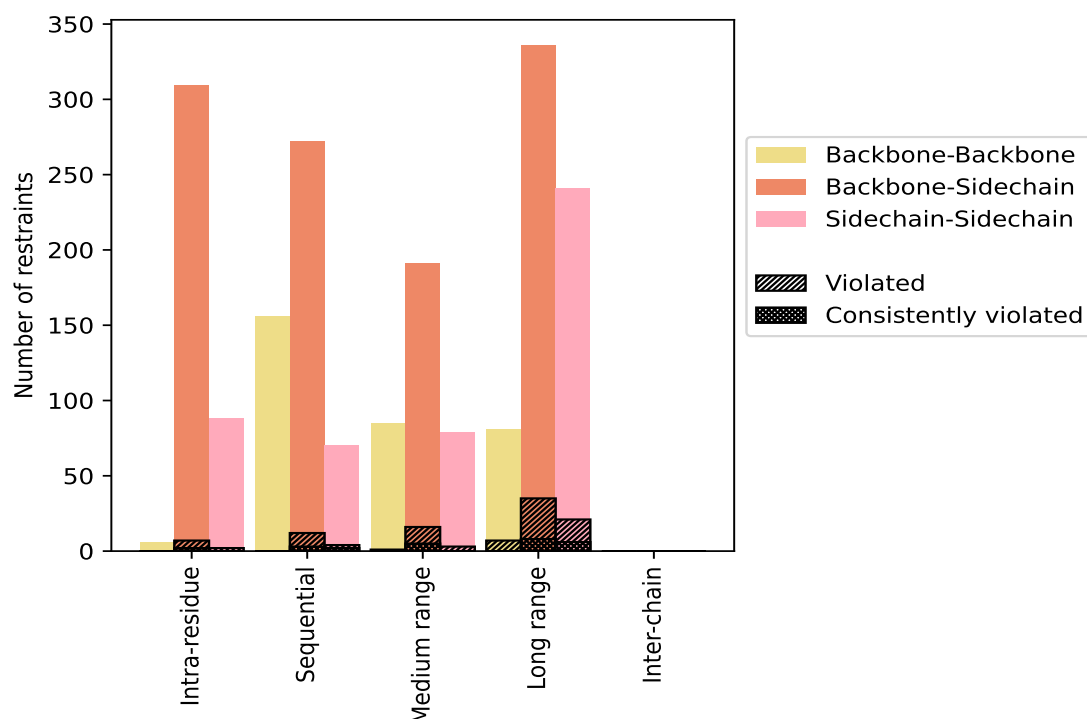
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                         | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|----------------------------------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                        |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| Intra-residue ( $ i-j =0$ )            | 403   | 21.1           | 9                     | 2.2            | 0.5            | 2                                  | 0.5            | 0.1            |
| Backbone-Backbone                      | 6     | 0.3            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 309   | 16.1           | 7                     | 2.3            | 0.4            | 2                                  | 0.6            | 0.1            |
| Sidechain-Sidechain                    | 88    | 4.6            | 2                     | 2.3            | 0.1            | 0                                  | 0.0            | 0.0            |
| Sequential ( $ i-j =1$ )               | 498   | 26.0           | 16                    | 3.2            | 0.8            | 5                                  | 1.0            | 0.3            |
| Backbone-Backbone                      | 156   | 8.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 272   | 14.2           | 12                    | 4.4            | 0.6            | 3                                  | 1.1            | 0.2            |
| Sidechain-Sidechain                    | 70    | 3.7            | 4                     | 5.7            | 0.2            | 2                                  | 2.9            | 0.1            |
| Medium range ( $ i-j >1$ & $ i-j <5$ ) | 339   | 17.7           | 15                    | 4.4            | 0.8            | 3                                  | 0.9            | 0.2            |
| Backbone-Backbone                      | 85    | 4.4            | 1                     | 1.2            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 175   | 9.1            | 11                    | 6.3            | 0.6            | 3                                  | 1.7            | 0.2            |
| Sidechain-Sidechain                    | 79    | 4.1            | 3                     | 3.8            | 0.2            | 0                                  | 0.0            | 0.0            |
| Long range ( $ i-j \geq 5$ )           | 646   | 33.8           | 61                    | 9.4            | 3.2            | 14                                 | 2.2            | 0.7            |
| Backbone-Backbone                      | 81    | 4.2            | 7                     | 8.6            | 0.4            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 324   | 16.9           | 33                    | 10.2           | 1.7            | 8                                  | 2.5            | 0.4            |
| Sidechain-Sidechain                    | 241   | 12.6           | 21                    | 8.7            | 1.1            | 6                                  | 2.5            | 0.3            |
| Inter-chain                            | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Hydrogen bond                          | 28    | 1.5            | 7                     | 25.0           | 0.4            | 2                                  | 7.1            | 0.1            |
| Disulfide bond                         | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total                                  | 1914  | 100.0          | 108                   | 5.6            | 5.6            | 26                                 | 1.4            | 1.4            |
| Backbone-Backbone                      | 328   | 17.1           | 8                     | 2.4            | 0.4            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 1108  | 57.9           | 70                    | 6.3            | 3.7            | 18                                 | 1.6            | 0.9            |
| Sidechain-Sidechain                    | 478   | 25.0           | 30                    | 6.3            | 1.6            | 8                                  | 1.7            | 0.4            |

<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        | 2                    | 9               | 12              | 31              | 0               | 54    | 0.83     | 3.53    | 1.01                | 0.24       |
| 2        | 2                    | 7               | 12              | 28              | 0               | 49    | 0.93     | 3.7     | 1.1                 | 0.25       |
| 3        | 2                    | 8               | 11              | 28              | 0               | 49    | 0.89     | 3.47    | 1.0                 | 0.31       |
| 4        | 3                    | 6               | 14              | 29              | 0               | 52    | 0.9      | 3.62    | 1.07                | 0.24       |
| 5        | 4                    | 8               | 12              | 30              | 0               | 54    | 0.8      | 3.37    | 0.95                | 0.26       |
| 6        | 5                    | 9               | 11              | 31              | 0               | 56    | 0.83     | 3.66    | 1.02                | 0.26       |
| 7        | 2                    | 5               | 12              | 27              | 0               | 46    | 1.01     | 3.64    | 1.09                | 0.34       |
| 8        | 2                    | 6               | 12              | 31              | 0               | 51    | 0.87     | 3.62    | 1.02                | 0.25       |
| 9        | 3                    | 10              | 11              | 32              | 0               | 56    | 0.78     | 3.43    | 0.97                | 0.24       |
| 10       | 4                    | 5               | 14              | 29              | 0               | 52    | 0.89     | 3.61    | 1.06                | 0.23       |

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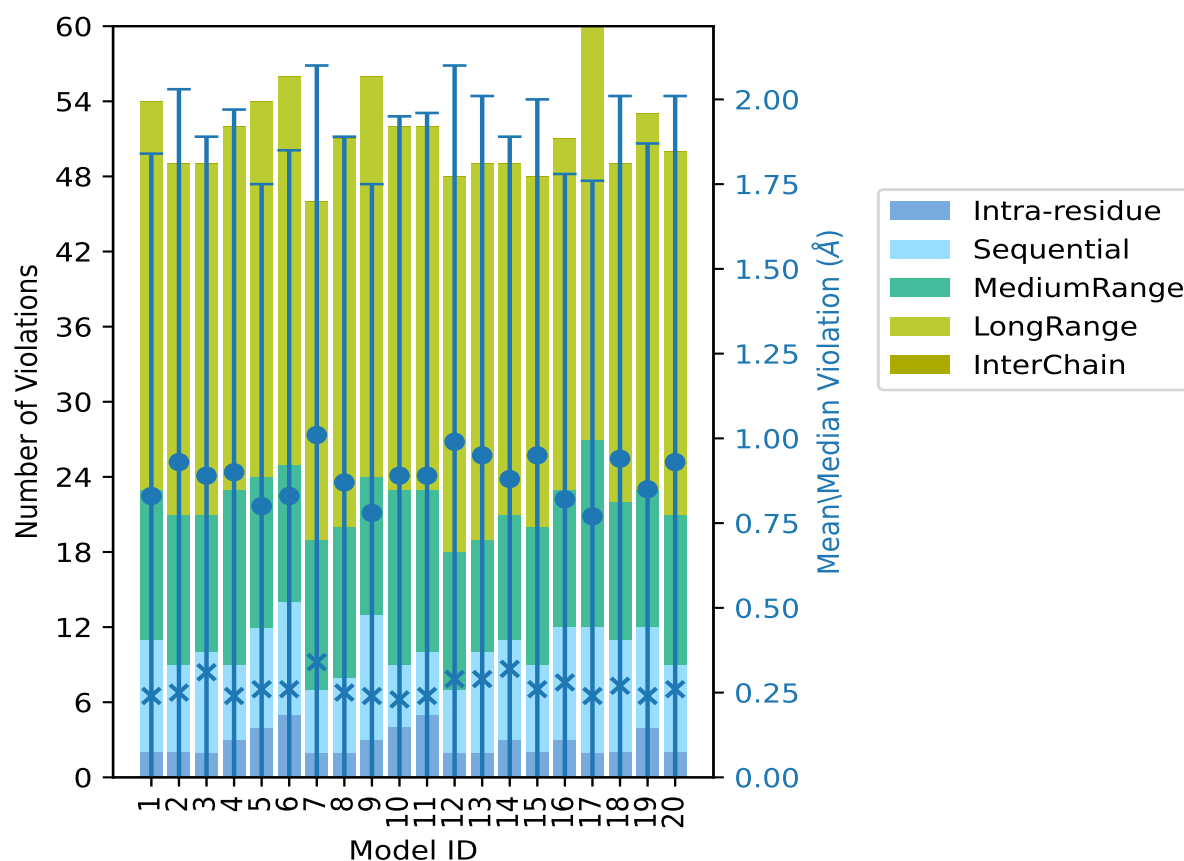
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 5                    | 5               | 13              | 29              | 0               | 52    | 0.89     | 3.62    | 1.07                | 0.24       |
| 12       | 2                    | 5               | 11              | 30              | 0               | 48    | 0.99     | 3.71    | 1.11                | 0.29       |
| 13       | 2                    | 8               | 9               | 30              | 0               | 49    | 0.95     | 3.6     | 1.06                | 0.29       |
| 14       | 3                    | 8               | 10              | 28              | 0               | 49    | 0.88     | 3.47    | 1.01                | 0.32       |
| 15       | 2                    | 7               | 11              | 28              | 0               | 48    | 0.95     | 3.53    | 1.05                | 0.26       |
| 16       | 3                    | 9               | 11              | 28              | 0               | 51    | 0.82     | 3.4     | 0.96                | 0.28       |
| 17       | 2                    | 10              | 15              | 33              | 0               | 60    | 0.77     | 3.52    | 0.99                | 0.24       |
| 18       | 2                    | 9               | 11              | 27              | 0               | 49    | 0.94     | 3.6     | 1.07                | 0.27       |
| 19       | 4                    | 8               | 11              | 30              | 0               | 53    | 0.85     | 3.58    | 1.02                | 0.24       |
| 20       | 2                    | 7               | 12              | 29              | 0               | 50    | 0.93     | 3.62    | 1.08                | 0.26       |

<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

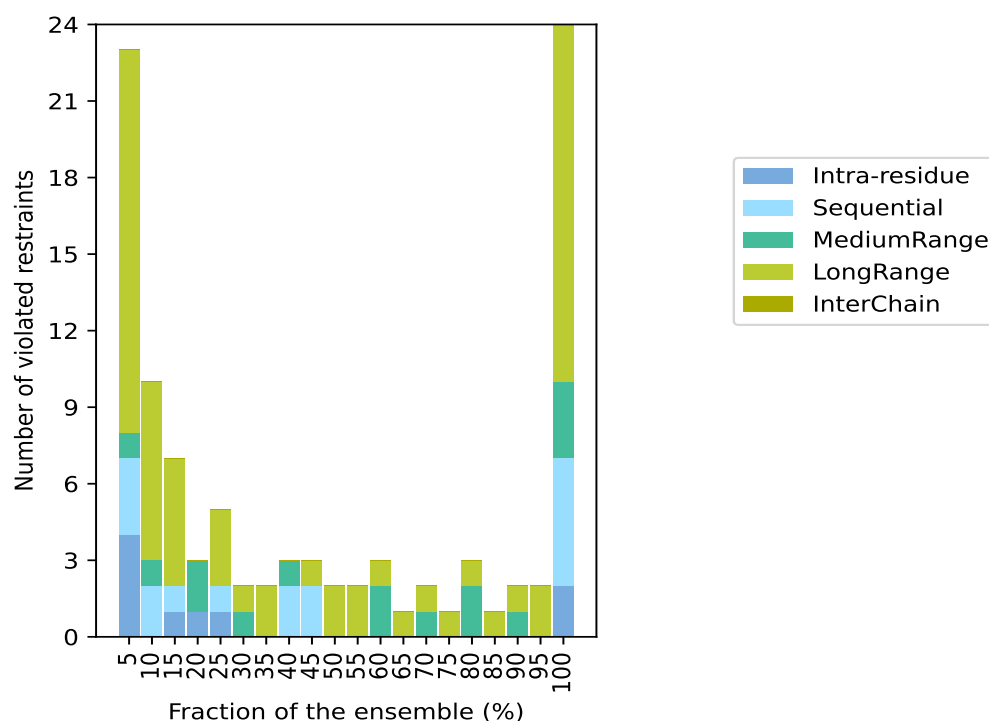
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1785(IR:394, SQ:482, MR:324, LR:585, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 4                             | 3               | 1               | 15              | 0               | 23    | 1                        | 5.0   |
| 0                             | 2               | 1               | 7               | 0               | 10    | 2                        | 10.0  |
| 1                             | 1               | 0               | 5               | 0               | 7     | 3                        | 15.0  |
| 1                             | 0               | 2               | 0               | 0               | 3     | 4                        | 20.0  |
| 1                             | 1               | 0               | 3               | 0               | 5     | 5                        | 25.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 6                        | 30.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 7                        | 35.0  |
| 0                             | 2               | 1               | 0               | 0               | 3     | 8                        | 40.0  |
| 0                             | 2               | 0               | 1               | 0               | 3     | 9                        | 45.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 10                       | 50.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 11                       | 55.0  |
| 0                             | 0               | 2               | 1               | 0               | 3     | 12                       | 60.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 13                       | 65.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 14                       | 70.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 15                       | 75.0  |
| 0                             | 0               | 2               | 1               | 0               | 3     | 16                       | 80.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 17                       | 85.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 18                       | 90.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 19                       | 95.0  |
| 2                             | 5               | 3               | 14              | 0               | 24    | 20                       | 100.0 |

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

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

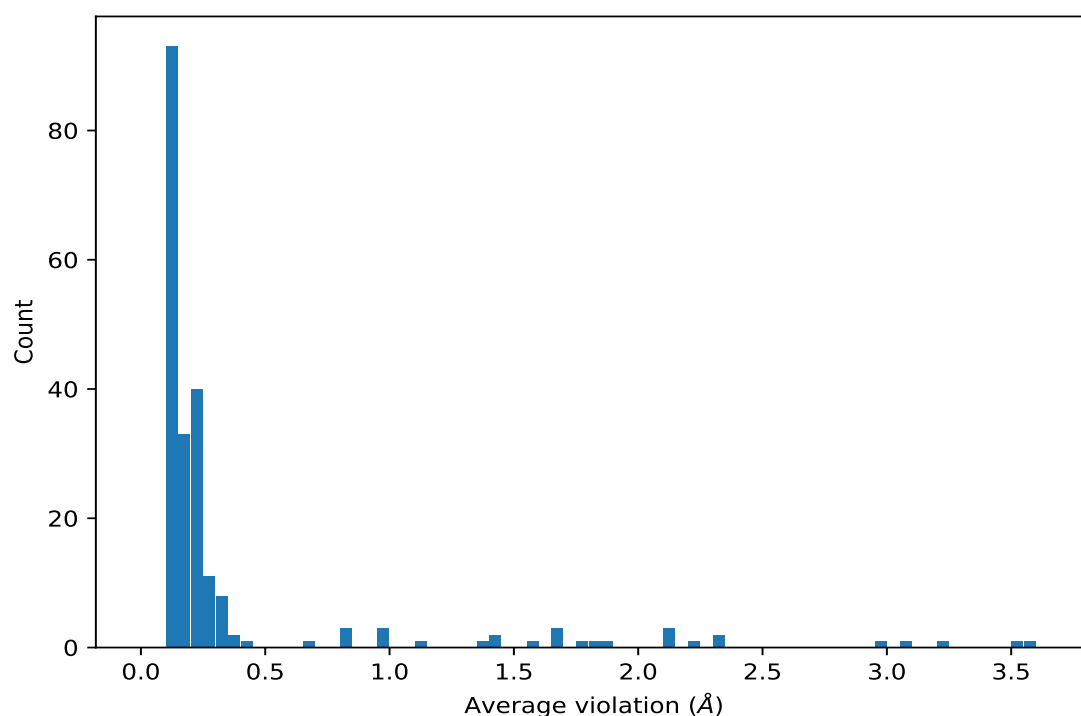
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,274)  | 1:9:A:TRP:H     | 1:14:A:TYR:HD1  | 20                  | 3.56     | 0.1                 | 3.59       |
| (1,275)  | 1:9:A:TRP:H     | 1:14:A:TYR:HE1  | 20                  | 3.53     | 0.09                | 3.56       |
| (1,807)  | 1:8:A:LYS:HA    | 1:14:A:TYR:HD1  | 20                  | 3.24     | 0.09                | 3.25       |
| (1,808)  | 1:8:A:LYS:HA    | 1:14:A:TYR:HE1  | 20                  | 3.05     | 0.1                 | 3.06       |
| (1,294)  | 1:12:A:GLN:H    | 1:14:A:TYR:HE1  | 20                  | 2.99     | 0.09                | 3.0        |
| (1,819)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HD1  | 20                  | 2.31     | 0.22                | 2.38       |
| (1,819)  | 1:9:A:TRP:HB2   | 1:14:A:TYR:HD1  | 20                  | 2.31     | 0.22                | 2.38       |
| (1,799)  | 1:7:A:VAL:HB    | 1:14:A:TYR:HD1  | 20                  | 2.23     | 0.73                | 2.76       |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD21 | 20                  | 2.12     | 0.1                 | 2.16       |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD22 | 20                  | 2.12     | 0.1                 | 2.16       |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD23 | 20                  | 2.12     | 0.1                 | 2.16       |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1  | 20                  | 1.89     | 0.25                | 1.95       |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA   | 20                  | 1.81     | 0.07                | 1.82       |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1  | 20                  | 1.75     | 0.03                | 1.75       |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1  | 20                  | 1.69     | 0.15                | 1.66       |
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1  | 20                  | 1.69     | 0.15                | 1.66       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1  | 20                  | 1.69     | 0.15                | 1.66       |
| (1,302)  | 1:14:A:TYR:H    | 1:14:A:TYR:HD1  | 20                  | 1.56     | 0.04                | 1.54       |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 20                  | 1.43     | 0.02                | 1.44       |
| (1,848)  | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1  | 20                  | 1.42     | 0.08                | 1.4        |
| (1,134)  | 1:31:A:PHE:HD1  | 1:33:A:LYS:H    | 20                  | 1.35     | 0.03                | 1.35       |
| (1,303)  | 1:14:A:TYR:H    | 1:14:A:TYR:HE1  | 20                  | 1.1      | 0.05                | 1.09       |
| (1,1116) | 1:14:A:TYR:HD1  | 1:36:A:THR:HG21 | 20                  | 0.99     | 0.28                | 1.08       |
| (1,1116) | 1:14:A:TYR:HD1  | 1:36:A:THR:HG22 | 20                  | 0.99     | 0.28                | 1.08       |
| (1,1116) | 1:14:A:TYR:HD1  | 1:36:A:THR:HG23 | 20                  | 0.99     | 0.28                | 1.08       |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H    | 20                  | 0.36     | 0.03                | 0.36       |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 20                  | 0.3      | 0.1                 | 0.27       |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 20                  | 0.3      | 0.1                 | 0.27       |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 20                  | 0.3      | 0.1                 | 0.27       |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA   | 20                  | 0.27     | 0.02                | 0.26       |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA   | 20                  | 0.27     | 0.02                | 0.26       |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA   | 20                  | 0.27     | 0.02                | 0.26       |
| (2,17)   | 1:27:A:ASP:O    | 1:31:A:PHE:H    | 20                  | 0.27     | 0.02                | 0.27       |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA   | 20                  | 0.22     | 0.05                | 0.2        |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA   | 20                  | 0.22     | 0.05                | 0.2        |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA   | 20                  | 0.22     | 0.05                | 0.2        |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA   | 20                  | 0.19     | 0.03                | 0.18       |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA   | 20                  | 0.19     | 0.03                | 0.18       |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 20                  | 0.19     | 0.03                | 0.18       |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 20                  | 0.19     | 0.03                | 0.18       |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 20                  | 0.19     | 0.03                | 0.18       |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 20                  | 0.19     | 0.03                | 0.18       |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 20                  | 0.15     | 0.02                | 0.15       |
| (1,731)  | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 20                  | 0.12     | 0.02                | 0.12       |
| (1,731)  | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 20                  | 0.12     | 0.02                | 0.12       |
| (1,1115) | 1:14:A:TYR:HE1  | 1:36:A:THR:HG21 | 19                  | 0.82     | 0.19                | 0.86       |
| (1,1115) | 1:14:A:TYR:HE1  | 1:36:A:THR:HG22 | 19                  | 0.82     | 0.19                | 0.86       |
| (1,1115) | 1:14:A:TYR:HE1  | 1:36:A:THR:HG23 | 19                  | 0.82     | 0.19                | 0.86       |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 19                  | 0.14     | 0.02                | 0.13       |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 19                  | 0.13     | 0.02                | 0.12       |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 19                  | 0.13     | 0.02                | 0.12       |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 19                  | 0.13     | 0.02                | 0.12       |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O    | 18                  | 0.39     | 0.05                | 0.41       |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 18                  | 0.18     | 0.04                | 0.18       |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 18                  | 0.18     | 0.04                | 0.18       |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 18                  | 0.18     | 0.04                | 0.18       |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 18                  | 0.18     | 0.04                | 0.18       |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 18                  | 0.18     | 0.04                | 0.18       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 18                  | 0.18     | 0.04                | 0.18       |
| (1,655)  | 1:74:A:MET:HA   | 1:76:A:GLY:H    | 18                  | 0.14     | 0.03                | 0.14       |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O    | 17                  | 0.2      | 0.03                | 0.21       |
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 17                  | 0.15     | 0.04                | 0.16       |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB   | 16                  | 0.22     | 0.05                | 0.21       |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB   | 16                  | 0.22     | 0.05                | 0.21       |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 16                  | 0.16     | 0.06                | 0.13       |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 16                  | 0.16     | 0.06                | 0.13       |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 16                  | 0.13     | 0.01                | 0.13       |
| (1,645)  | 1:44:A:LYS:H    | 1:75:A:MET:H    | 15                  | 0.14     | 0.02                | 0.14       |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 14                  | 0.24     | 0.01                | 0.24       |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 14                  | 0.24     | 0.01                | 0.24       |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 14                  | 0.24     | 0.01                | 0.24       |
| (1,972)  | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 14                  | 0.12     | 0.02                | 0.12       |
| (1,972)  | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 14                  | 0.12     | 0.02                | 0.12       |
| (1,972)  | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 14                  | 0.12     | 0.02                | 0.12       |
| (1,585)  | 1:5:A:ILE:HD11  | 1:66:A:LEU:H    | 13                  | 0.12     | 0.01                | 0.12       |
| (1,585)  | 1:5:A:ILE:HD12  | 1:66:A:LEU:H    | 13                  | 0.12     | 0.01                | 0.12       |
| (1,585)  | 1:5:A:ILE:HD13  | 1:66:A:LEU:H    | 13                  | 0.12     | 0.01                | 0.12       |
| (1,844)  | 1:12:A:GLN:HG2  | 1:14:A:TYR:HE1  | 12                  | 0.23     | 0.07                | 0.23       |
| (1,844)  | 1:12:A:GLN:HG3  | 1:14:A:TYR:HE1  | 12                  | 0.23     | 0.07                | 0.23       |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD11 | 12                  | 0.14     | 0.03                | 0.12       |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD12 | 12                  | 0.14     | 0.03                | 0.12       |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD13 | 12                  | 0.14     | 0.03                | 0.12       |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG21 | 12                  | 0.13     | 0.02                | 0.13       |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG22 | 12                  | 0.13     | 0.02                | 0.13       |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG23 | 12                  | 0.13     | 0.02                | 0.13       |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG21 | 12                  | 0.13     | 0.02                | 0.13       |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG22 | 12                  | 0.13     | 0.02                | 0.13       |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG23 | 12                  | 0.13     | 0.02                | 0.13       |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG21 | 12                  | 0.13     | 0.02                | 0.13       |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG22 | 12                  | 0.13     | 0.02                | 0.13       |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG23 | 12                  | 0.13     | 0.02                | 0.13       |
| (1,1125) | 1:33:A:LYS:HB2  | 1:38:A:VAL:HB   | 11                  | 0.67     | 0.01                | 0.66       |
| (1,1127) | 1:33:A:LYS:HD3  | 1:38:A:VAL:HB   | 11                  | 0.15     | 0.02                | 0.14       |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB2  | 10                  | 0.33     | 0.08                | 0.35       |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB3  | 10                  | 0.33     | 0.08                | 0.35       |
| (1,252)  | 1:7:A:VAL:H     | 1:32:A:LEU:HB2  | 10                  | 0.14     | 0.02                | 0.14       |
| (1,287)  | 1:13:A:GLU:H    | 1:14:A:TYR:HE1  | 9                   | 0.4      | 0.15                | 0.35       |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD2  | 9                   | 0.26     | 0.08                | 0.22       |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD3  | 9                   | 0.26     | 0.08                | 0.22       |
| (1,744)  | 1:2:A:ALA:HA    | 1:3:A:LEU:HG    | 9                   | 0.16     | 0.02                | 0.15       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,288)  | 1:13:A:GLU:H    | 1:14:A:TYR:HD1  | 8                   | 0.31     | 0.1                 | 0.27       |
| (1,1482) | 1:68:A:PRO:HA   | 1:70:A:THR:HB   | 8                   | 0.11     | 0.0                 | 0.11       |
| (1,756)  | 1:4:A:PRO:HD2   | 1:5:A:ILE:HA    | 8                   | 0.1      | 0.0                 | 0.1        |
| (1,756)  | 1:4:A:PRO:HD3   | 1:5:A:ILE:HA    | 8                   | 0.1      | 0.0                 | 0.1        |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG2  | 7                   | 0.28     | 0.08                | 0.31       |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG3  | 7                   | 0.28     | 0.08                | 0.31       |
| (1,1264) | 1:59:A:VAL:HA   | 1:64:A:LEU:HG   | 7                   | 0.13     | 0.03                | 0.12       |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA2  | 6                   | 0.18     | 0.07                | 0.16       |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA3  | 6                   | 0.18     | 0.07                | 0.16       |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA2  | 6                   | 0.18     | 0.07                | 0.16       |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA3  | 6                   | 0.18     | 0.07                | 0.16       |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA2  | 6                   | 0.18     | 0.07                | 0.16       |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA3  | 6                   | 0.18     | 0.07                | 0.16       |
| (1,1317) | 1:61:A:LEU:HA   | 1:64:A:LEU:HG   | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1407) | 1:73:A:MET:HB2  | 1:74:A:MET:HG3  | 5                   | 0.2      | 0.02                | 0.19       |
| (1,1407) | 1:73:A:MET:HB3  | 1:74:A:MET:HG3  | 5                   | 0.2      | 0.02                | 0.19       |
| (1,1694) | 1:38:A:VAL:HG11 | 1:43:A:GLN:H    | 5                   | 0.13     | 0.02                | 0.14       |
| (1,1694) | 1:38:A:VAL:HG12 | 1:43:A:GLN:H    | 5                   | 0.13     | 0.02                | 0.14       |
| (1,1694) | 1:38:A:VAL:HG13 | 1:43:A:GLN:H    | 5                   | 0.13     | 0.02                | 0.14       |
| (1,1694) | 1:38:A:VAL:HG21 | 1:43:A:GLN:H    | 5                   | 0.13     | 0.02                | 0.14       |
| (1,1694) | 1:38:A:VAL:HG22 | 1:43:A:GLN:H    | 5                   | 0.13     | 0.02                | 0.14       |
| (1,1694) | 1:38:A:VAL:HG23 | 1:43:A:GLN:H    | 5                   | 0.13     | 0.02                | 0.14       |
| (1,597)  | 1:4:A:PRO:HG2   | 1:69:A:ASN:H    | 5                   | 0.11     | 0.01                | 0.11       |
| (1,210)  | 1:26:A:LEU:H    | 1:26:A:LEU:HB2  | 5                   | 0.1      | 0.0                 | 0.1        |
| (1,591)  | 1:5:A:ILE:HD11  | 1:67:A:LYS:H    | 5                   | 0.1      | 0.0                 | 0.1        |
| (1,591)  | 1:5:A:ILE:HD12  | 1:67:A:LYS:H    | 5                   | 0.1      | 0.0                 | 0.1        |
| (1,591)  | 1:5:A:ILE:HD13  | 1:67:A:LYS:H    | 5                   | 0.1      | 0.0                 | 0.1        |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG11 | 4                   | 0.24     | 0.01                | 0.24       |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG12 | 4                   | 0.24     | 0.01                | 0.24       |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG13 | 4                   | 0.24     | 0.01                | 0.24       |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG21 | 4                   | 0.24     | 0.01                | 0.24       |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG22 | 4                   | 0.24     | 0.01                | 0.24       |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG23 | 4                   | 0.24     | 0.01                | 0.24       |
| (1,1687) | 1:38:A:VAL:HG11 | 1:40:A:PRO:HA   | 4                   | 0.14     | 0.03                | 0.14       |
| (1,1687) | 1:38:A:VAL:HG12 | 1:40:A:PRO:HA   | 4                   | 0.14     | 0.03                | 0.14       |
| (1,1687) | 1:38:A:VAL:HG13 | 1:40:A:PRO:HA   | 4                   | 0.14     | 0.03                | 0.14       |
| (1,1687) | 1:38:A:VAL:HG21 | 1:40:A:PRO:HA   | 4                   | 0.14     | 0.03                | 0.14       |
| (1,1687) | 1:38:A:VAL:HG22 | 1:40:A:PRO:HA   | 4                   | 0.14     | 0.03                | 0.14       |
| (1,1687) | 1:38:A:VAL:HG23 | 1:40:A:PRO:HA   | 4                   | 0.14     | 0.03                | 0.14       |
| (1,983)  | 1:26:A:LEU:HA   | 1:26:A:LEU:HG   | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,1121) | 1:38:A:VAL:HA   | 1:78:A:ARG:HD2  | 3                   | 0.31     | 0.08                | 0.36       |
| (1,1121) | 1:38:A:VAL:HA   | 1:78:A:ARG:HD3  | 3                   | 0.31     | 0.08                | 0.36       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1436) | 1:77:A:THR:HB   | 1:78:A:ARG:HD2  | 3                   | 0.22     | 0.06                | 0.25       |
| (1,1436) | 1:77:A:THR:HB   | 1:78:A:ARG:HD3  | 3                   | 0.22     | 0.06                | 0.25       |
| (1,232)  | 1:38:A:VAL:HB   | 1:79:A:GLU:H    | 3                   | 0.2      | 0.01                | 0.21       |
| (1,626)  | 1:45:A:LEU:HA   | 1:73:A:MET:H    | 3                   | 0.13     | 0.02                | 0.14       |
| (1,1699) | 1:38:A:VAL:HG11 | 1:76:A:GLY:HA2  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,1699) | 1:38:A:VAL:HG11 | 1:76:A:GLY:HA3  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,1699) | 1:38:A:VAL:HG12 | 1:76:A:GLY:HA2  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,1699) | 1:38:A:VAL:HG12 | 1:76:A:GLY:HA3  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,1699) | 1:38:A:VAL:HG13 | 1:76:A:GLY:HA2  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,1699) | 1:38:A:VAL:HG13 | 1:76:A:GLY:HA3  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,1699) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA2  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,1699) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA3  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,1699) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA2  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,1699) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA3  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,1699) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA2  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,1699) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA3  | 3                   | 0.13     | 0.02                | 0.13       |
| (1,462)  | 1:45:A:LEU:H    | 1:45:A:LEU:HD21 | 3                   | 0.13     | 0.01                | 0.12       |
| (1,462)  | 1:45:A:LEU:H    | 1:45:A:LEU:HD22 | 3                   | 0.13     | 0.01                | 0.12       |
| (1,462)  | 1:45:A:LEU:H    | 1:45:A:LEU:HD23 | 3                   | 0.13     | 0.01                | 0.12       |
| (1,1287) | 1:24:A:THR:HA   | 1:61:A:LEU:HA   | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1131) | 1:38:A:VAL:HG21 | 1:74:A:MET:HB3  | 2                   | 0.26     | 0.01                | 0.26       |
| (1,1131) | 1:38:A:VAL:HG22 | 1:74:A:MET:HB3  | 2                   | 0.26     | 0.01                | 0.26       |
| (1,1131) | 1:38:A:VAL:HG23 | 1:74:A:MET:HB3  | 2                   | 0.26     | 0.01                | 0.26       |
| (1,1702) | 1:38:A:VAL:HG11 | 1:77:A:THR:HG21 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG11 | 1:77:A:THR:HG22 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG11 | 1:77:A:THR:HG23 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG12 | 1:77:A:THR:HG21 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG12 | 1:77:A:THR:HG22 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG12 | 1:77:A:THR:HG23 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG13 | 1:77:A:THR:HG21 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG13 | 1:77:A:THR:HG22 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG13 | 1:77:A:THR:HG23 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG21 | 1:77:A:THR:HG21 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG21 | 1:77:A:THR:HG22 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG21 | 1:77:A:THR:HG23 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG22 | 1:77:A:THR:HG21 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG22 | 1:77:A:THR:HG22 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG22 | 1:77:A:THR:HG23 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG23 | 1:77:A:THR:HG21 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG23 | 1:77:A:THR:HG22 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1702) | 1:38:A:VAL:HG23 | 1:77:A:THR:HG23 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1722) | 1:44:A:LYS:HG2  | 1:45:A:LEU:H    | 2                   | 0.19     | 0.06                | 0.19       |

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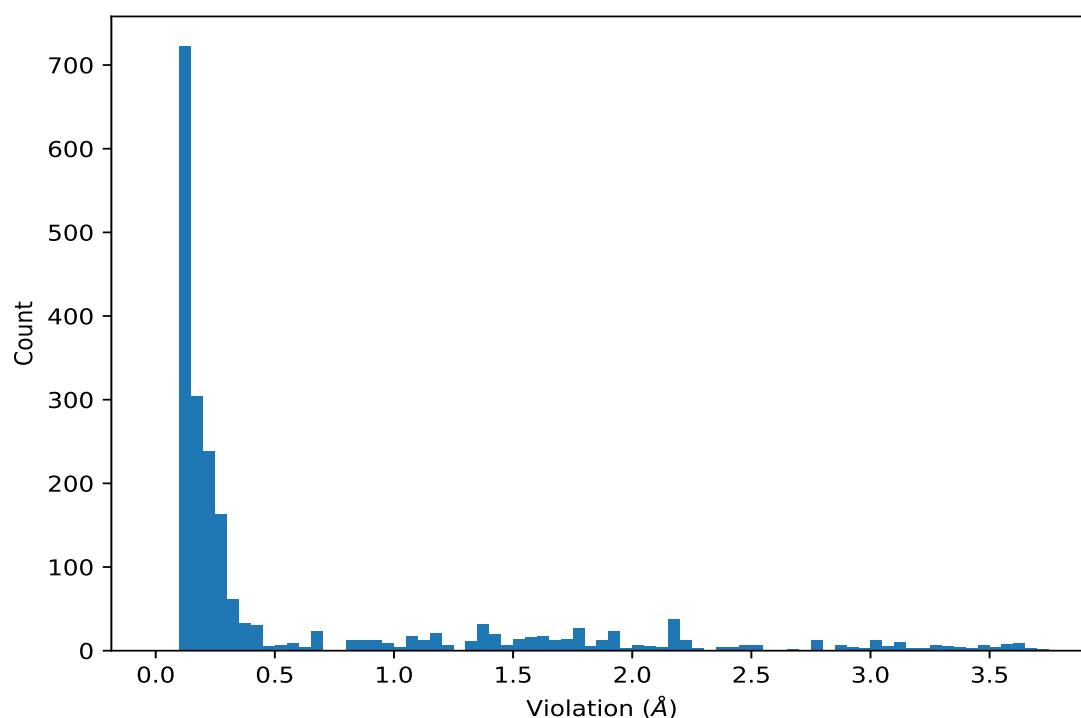
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1722) | 1:44:A:LYS:HG3  | 1:45:A:LEU:H    | 2                   | 0.19     | 0.06                | 0.19       |
| (1,1698) | 1:38:A:VAL:HG11 | 1:76:A:GLY:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1698) | 1:38:A:VAL:HG12 | 1:76:A:GLY:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1698) | 1:38:A:VAL:HG13 | 1:76:A:GLY:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1698) | 1:38:A:VAL:HG21 | 1:76:A:GLY:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1698) | 1:38:A:VAL:HG22 | 1:76:A:GLY:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1698) | 1:38:A:VAL:HG23 | 1:76:A:GLY:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,454)  | 1:29:A:LYS:HE2  | 1:45:A:LEU:H    | 2                   | 0.16     | 0.05                | 0.16       |
| (1,1549) | 1:8:A:LYS:HE2   | 1:9:A:TRP:H     | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1549) | 1:8:A:LYS:HE3   | 1:9:A:TRP:H     | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1705) | 1:38:A:VAL:HG11 | 1:78:A:ARG:HG2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1705) | 1:38:A:VAL:HG11 | 1:78:A:ARG:HG3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1705) | 1:38:A:VAL:HG12 | 1:78:A:ARG:HG2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1705) | 1:38:A:VAL:HG12 | 1:78:A:ARG:HG3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1705) | 1:38:A:VAL:HG13 | 1:78:A:ARG:HG2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1705) | 1:38:A:VAL:HG13 | 1:78:A:ARG:HG3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1705) | 1:38:A:VAL:HG21 | 1:78:A:ARG:HG2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1705) | 1:38:A:VAL:HG21 | 1:78:A:ARG:HG3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1705) | 1:38:A:VAL:HG22 | 1:78:A:ARG:HG2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1705) | 1:38:A:VAL:HG22 | 1:78:A:ARG:HG3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1705) | 1:38:A:VAL:HG23 | 1:78:A:ARG:HG2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1705) | 1:38:A:VAL:HG23 | 1:78:A:ARG:HG3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,50)   | 1:19:A:LEU:HG   | 1:24:A:THR:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1689) | 1:38:A:VAL:HG11 | 1:42:A:ARG:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1689) | 1:38:A:VAL:HG12 | 1:42:A:ARG:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1689) | 1:38:A:VAL:HG13 | 1:42:A:ARG:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1689) | 1:38:A:VAL:HG21 | 1:42:A:ARG:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1689) | 1:38:A:VAL:HG22 | 1:42:A:ARG:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1689) | 1:38:A:VAL:HG23 | 1:42:A:ARG:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,269)  | 1:8:A:LYS:H     | 1:32:A:LEU:HD21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,269)  | 1:8:A:LYS:H     | 1:32:A:LEU:HD22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,269)  | 1:8:A:LYS:H     | 1:32:A:LEU:HD23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,18)   | 1:27:A:ASP:O    | 1:31:A:PHE:N    | 2                   | 0.1      | 0.0                 | 0.1        |

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

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

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

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



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

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

| Key     | Atom-1      | Atom-2         | Model ID | Violation (Å) |
|---------|-------------|----------------|----------|---------------|
| (1,274) | 1:9:A:TRP:H | 1:14:A:TYR:HD1 | 12       | 3.71          |
| (1,274) | 1:9:A:TRP:H | 1:14:A:TYR:HD1 | 2        | 3.7           |
| (1,275) | 1:9:A:TRP:H | 1:14:A:TYR:HE1 | 12       | 3.68          |
| (1,275) | 1:9:A:TRP:H | 1:14:A:TYR:HE1 | 2        | 3.66          |
| (1,275) | 1:9:A:TRP:H | 1:14:A:TYR:HE1 | 6        | 3.66          |
| (1,274) | 1:9:A:TRP:H | 1:14:A:TYR:HD1 | 7        | 3.64          |
| (1,274) | 1:9:A:TRP:H | 1:14:A:TYR:HD1 | 4        | 3.62          |
| (1,274) | 1:9:A:TRP:H | 1:14:A:TYR:HD1 | 8        | 3.62          |
| (1,274) | 1:9:A:TRP:H | 1:14:A:TYR:HD1 | 11       | 3.62          |
| (1,274) | 1:9:A:TRP:H | 1:14:A:TYR:HD1 | 20       | 3.62          |
| (1,274) | 1:9:A:TRP:H | 1:14:A:TYR:HD1 | 10       | 3.61          |
| (1,275) | 1:9:A:TRP:H | 1:14:A:TYR:HE1 | 7        | 3.6           |
| (1,274) | 1:9:A:TRP:H | 1:14:A:TYR:HD1 | 13       | 3.6           |
| (1,274) | 1:9:A:TRP:H | 1:14:A:TYR:HD1 | 18       | 3.6           |
| (1,275) | 1:9:A:TRP:H | 1:14:A:TYR:HE1 | 20       | 3.59          |
| (1,275) | 1:9:A:TRP:H | 1:14:A:TYR:HE1 | 4        | 3.58          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 8        | 3.58          |
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 11       | 3.58          |
| (1,274) | 1:9:A:TRP:H  | 1:14:A:TYR:HD1 | 6        | 3.58          |
| (1,274) | 1:9:A:TRP:H  | 1:14:A:TYR:HD1 | 19       | 3.58          |
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 10       | 3.57          |
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 13       | 3.56          |
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 18       | 3.55          |
| (1,274) | 1:9:A:TRP:H  | 1:14:A:TYR:HD1 | 1        | 3.53          |
| (1,274) | 1:9:A:TRP:H  | 1:14:A:TYR:HD1 | 15       | 3.53          |
| (1,274) | 1:9:A:TRP:H  | 1:14:A:TYR:HD1 | 17       | 3.52          |
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 15       | 3.49          |
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 19       | 3.49          |
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 3        | 3.47          |
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 14       | 3.47          |
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 17       | 3.46          |
| (1,274) | 1:9:A:TRP:H  | 1:14:A:TYR:HD1 | 14       | 3.46          |
| (1,274) | 1:9:A:TRP:H  | 1:14:A:TYR:HD1 | 3        | 3.45          |
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 9        | 3.43          |
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 1        | 3.42          |
| (1,274) | 1:9:A:TRP:H  | 1:14:A:TYR:HD1 | 9        | 3.41          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 6        | 3.4           |
| (1,274) | 1:9:A:TRP:H  | 1:14:A:TYR:HD1 | 16       | 3.4           |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 2        | 3.39          |
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 5        | 3.37          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 12       | 3.34          |
| (1,275) | 1:9:A:TRP:H  | 1:14:A:TYR:HE1 | 16       | 3.33          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 11       | 3.32          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 20       | 3.31          |
| (1,274) | 1:9:A:TRP:H  | 1:14:A:TYR:HD1 | 5        | 3.31          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 7        | 3.3           |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 6        | 3.29          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 10       | 3.29          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 18       | 3.27          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 8        | 3.26          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 4        | 3.25          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 14       | 3.25          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 13       | 3.24          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 6        | 3.21          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 9        | 3.2           |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 3        | 3.19          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 15       | 3.19          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 2        | 3.18          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 19       | 3.15          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 8        | 3.15          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 12       | 3.14          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 5        | 3.14          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 17       | 3.14          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 20       | 3.11          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 1        | 3.11          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 2        | 3.11          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 11       | 3.1           |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 14       | 3.1           |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 7        | 3.09          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 10       | 3.08          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 8        | 3.07          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 18       | 3.06          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 20       | 3.06          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 3        | 3.05          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 4        | 3.05          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 9        | 3.04          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 13       | 3.04          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 12       | 3.04          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 19       | 3.04          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 4        | 3.03          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 5        | 3.02          |
| (1,807) | 1:8:A:LYS:HA | 1:14:A:TYR:HD1 | 16       | 3.02          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 7        | 3.01          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 11       | 3.01          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 10       | 3.0           |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 18       | 3.0           |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 15       | 2.99          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 14       | 2.99          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 15       | 2.96          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 17       | 2.93          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 19       | 2.93          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 5        | 2.93          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 1        | 2.92          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 3        | 2.9           |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 13       | 2.9           |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 9        | 2.89          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 16       | 2.89          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 1        | 2.87          |
| (1,808) | 1:8:A:LYS:HA | 1:14:A:TYR:HE1 | 16       | 2.86          |
| (1,294) | 1:12:A:GLN:H | 1:14:A:TYR:HE1 | 17       | 2.81          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 11       | 2.78          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 1        | 2.77          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 2        | 2.77          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 4        | 2.77          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 10       | 2.77          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 15       | 2.77          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 18       | 2.77          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 20       | 2.77          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 7        | 2.76          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 13       | 2.76          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 17       | 2.76          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 12       | 2.75          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 19       | 2.75          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 12       | 2.66          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 12       | 2.66          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 20       | 2.55          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 20       | 2.55          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 4        | 2.53          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 4        | 2.53          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 7        | 2.53          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 7        | 2.53          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 13       | 2.46          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 13       | 2.46          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 2        | 2.45          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 2        | 2.45          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 11       | 2.45          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 11       | 2.45          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 18       | 2.44          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 18       | 2.44          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 10       | 2.43          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 10       | 2.43          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 15       | 2.38          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 15       | 2.38          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 17       | 2.37          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 17       | 2.37          |
| (1,818)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HE1  | 12       | 2.26          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 6        | 2.25          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 6        | 2.25          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD21 | 16       | 2.24          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD22 | 16       | 2.24          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD23 | 16       | 2.24          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD21 | 13       | 2.23          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD22 | 13       | 2.23          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD23 | 13       | 2.23          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 8        | 2.21          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 8        | 2.21          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 9        | 2.21          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 9        | 2.21          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD21 | 18       | 2.2           |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD22 | 18       | 2.2           |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD23 | 18       | 2.2           |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD21 | 10       | 2.19          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD22 | 10       | 2.19          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD23 | 10       | 2.19          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD21 | 20       | 2.19          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD22 | 20       | 2.19          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD23 | 20       | 2.19          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD21 | 4        | 2.18          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD22 | 4        | 2.18          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD23 | 4        | 2.18          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD21 | 11       | 2.18          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD22 | 11       | 2.18          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD23 | 11       | 2.18          |
| (1,819)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HD1  | 1        | 2.18          |
| (1,819)  | 1:9:A:TRP:HB2  | 1:14:A:TYR:HD1  | 1        | 2.18          |
| (1,818)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HE1  | 20       | 2.18          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD21 | 1        | 2.17          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD22 | 1        | 2.17          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD23 | 1        | 2.17          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD21 | 7        | 2.17          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD22 | 7        | 2.17          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD23 | 7        | 2.17          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD21 | 12       | 2.17          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD22 | 12       | 2.17          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD23 | 12       | 2.17          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD21 | 2        | 2.16          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD22 | 2        | 2.16          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD23 | 2        | 2.16          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD21 | 15       | 2.16          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD22 | 15       | 2.16          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD23 | 15       | 2.16          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD21 | 17       | 2.16          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD22 | 17       | 2.16          |
| (1,1452) | 1:31:A:PHE:HD1 | 1:32:A:LEU:HD23 | 17       | 2.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,819)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HD1  | 3        | 2.16          |
| (1,819)  | 1:9:A:TRP:HB2   | 1:14:A:TYR:HD1  | 3        | 2.16          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD21 | 19       | 2.15          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD22 | 19       | 2.15          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD23 | 19       | 2.15          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1  | 7        | 2.12          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1  | 4        | 2.11          |
| (1,819)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HD1  | 19       | 2.1           |
| (1,819)  | 1:9:A:TRP:HB2   | 1:14:A:TYR:HD1  | 19       | 2.1           |
| (1,819)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HD1  | 14       | 2.09          |
| (1,819)  | 1:9:A:TRP:HB2   | 1:14:A:TYR:HD1  | 14       | 2.09          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD21 | 14       | 2.07          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD22 | 14       | 2.07          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD23 | 14       | 2.07          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1  | 13       | 2.05          |
| (1,819)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HD1  | 5        | 2.04          |
| (1,819)  | 1:9:A:TRP:HB2   | 1:14:A:TYR:HD1  | 5        | 2.04          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1  | 18       | 2.04          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1  | 11       | 2.03          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1  | 2        | 2.02          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1  | 10       | 2.02          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD21 | 9        | 1.97          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD22 | 9        | 1.97          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD23 | 9        | 1.97          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD21 | 6        | 1.95          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD22 | 6        | 1.95          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD23 | 6        | 1.95          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD21 | 8        | 1.95          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD22 | 8        | 1.95          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD23 | 8        | 1.95          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1  | 15       | 1.95          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1  | 17       | 1.95          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD21 | 3        | 1.94          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD22 | 3        | 1.94          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD23 | 3        | 1.94          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD21 | 5        | 1.94          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD22 | 5        | 1.94          |
| (1,1452) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HD23 | 5        | 1.94          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1  | 18       | 1.94          |
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1  | 18       | 1.94          |
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1  | 18       | 1.94          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1  | 9        | 1.93          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 9        | 1.93          |
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 9        | 1.93          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 19       | 1.92          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1 | 6        | 1.92          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 6        | 1.91          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 3        | 1.9           |
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 3        | 1.9           |
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 3        | 1.9           |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 13       | 1.88          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 4        | 1.87          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 17       | 1.86          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 1        | 1.85          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 10       | 1.85          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 12       | 1.85          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 16       | 1.85          |
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 16       | 1.85          |
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 16       | 1.85          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1 | 9        | 1.85          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 15       | 1.84          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 7        | 1.83          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 8        | 1.8           |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 14       | 1.8           |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 6        | 1.8           |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 5        | 1.79          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 20       | 1.79          |
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 20       | 1.79          |
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 20       | 1.79          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 14       | 1.79          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 11       | 1.78          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 8        | 1.78          |
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 8        | 1.78          |
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 8        | 1.78          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 14       | 1.78          |
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 14       | 1.78          |
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 14       | 1.78          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1 | 3        | 1.78          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 19       | 1.78          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 5        | 1.77          |
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 5        | 1.77          |
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 5        | 1.77          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 2        | 1.77          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 15       | 1.77          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 20       | 1.77          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1 | 8        | 1.76          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 1        | 1.76          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 4        | 1.76          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 11       | 1.76          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 9        | 1.75          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 10       | 1.75          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 12       | 1.75          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 3        | 1.74          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 7        | 1.74          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 13       | 1.74          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 17       | 1.74          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 2        | 1.73          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 2        | 1.73          |
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 2        | 1.73          |
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 2        | 1.73          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 3        | 1.73          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 16       | 1.73          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 18       | 1.73          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 20       | 1.71          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 5        | 1.71          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 8        | 1.71          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1 | 1        | 1.7           |
| (1,302)  | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 6        | 1.7           |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 16       | 1.69          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1 | 5        | 1.69          |
| (1,1047) | 1:31:A:PHE:HD1  | 1:32:A:LEU:HA  | 18       | 1.68          |
| (1,819)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HD1 | 16       | 1.68          |
| (1,819)  | 1:9:A:TRP:HB2   | 1:14:A:TYR:HD1 | 16       | 1.68          |
| (1,818)  | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1 | 14       | 1.68          |
| (1,248)  | 1:7:A:VAL:H     | 1:14:A:TYR:HD1 | 9        | 1.68          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 11       | 1.67          |
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 11       | 1.67          |
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 11       | 1.67          |
| (1,848)  | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1 | 6        | 1.66          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 6        | 1.65          |
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 6        | 1.65          |
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 6        | 1.65          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 12       | 1.65          |
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 12       | 1.65          |
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 12       | 1.65          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 7        | 1.64          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,885) | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 7        | 1.64          |
| (1,885) | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 7        | 1.64          |
| (1,885) | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 1        | 1.62          |
| (1,885) | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 1        | 1.62          |
| (1,885) | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 1        | 1.62          |
| (1,885) | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 15       | 1.61          |
| (1,885) | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 15       | 1.61          |
| (1,885) | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 15       | 1.61          |
| (1,818) | 1:9:A:TRP:HB3   | 1:14:A:TYR:HE1 | 19       | 1.61          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 14       | 1.6           |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 5        | 1.59          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 8        | 1.59          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 16       | 1.59          |
| (1,885) | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 4        | 1.57          |
| (1,885) | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 4        | 1.57          |
| (1,885) | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 4        | 1.57          |
| (1,885) | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 10       | 1.57          |
| (1,885) | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 10       | 1.57          |
| (1,885) | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 10       | 1.57          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 2        | 1.57          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 12       | 1.57          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 20       | 1.57          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 17       | 1.56          |
| (1,885) | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 17       | 1.55          |
| (1,885) | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 17       | 1.55          |
| (1,885) | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 17       | 1.55          |
| (1,848) | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1 | 14       | 1.54          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 1        | 1.54          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 3        | 1.54          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 7        | 1.54          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 11       | 1.54          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 13       | 1.54          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 4        | 1.53          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 10       | 1.53          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 18       | 1.53          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 19       | 1.53          |
| (1,885) | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1 | 13       | 1.52          |
| (1,885) | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1 | 13       | 1.52          |
| (1,885) | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1 | 13       | 1.52          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 9        | 1.51          |
| (1,302) | 1:14:A:TYR:H    | 1:14:A:TYR:HD1 | 15       | 1.49          |
| (1,848) | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1 | 5        | 1.48          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,848)  | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1  | 2        | 1.46          |
| (1,848)  | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1  | 3        | 1.46          |
| (1,848)  | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1  | 16       | 1.46          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 6        | 1.46          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 17       | 1.46          |
| (1,799)  | 1:7:A:VAL:HB    | 1:14:A:TYR:HD1  | 16       | 1.45          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 4        | 1.45          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 8        | 1.45          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 13       | 1.45          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 19       | 1.45          |
| (1,848)  | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1  | 8        | 1.44          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 5        | 1.44          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 10       | 1.44          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 12       | 1.44          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 14       | 1.44          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 15       | 1.44          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 1        | 1.43          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 7        | 1.43          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 9        | 1.43          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 2        | 1.42          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 3        | 1.42          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 11       | 1.42          |
| (1,848)  | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1  | 12       | 1.41          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 16       | 1.41          |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 20       | 1.41          |
| (1,848)  | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1  | 9        | 1.4           |
| (1,848)  | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1  | 11       | 1.4           |
| (1,848)  | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1  | 20       | 1.4           |
| (1,134)  | 1:31:A:PHE:HD1  | 1:33:A:LYS:H    | 19       | 1.4           |
| (1,117)  | 1:31:A:PHE:HD1  | 1:32:A:LEU:H    | 18       | 1.4           |
| (1,134)  | 1:31:A:PHE:HD1  | 1:33:A:LYS:H    | 6        | 1.39          |
| (1,134)  | 1:31:A:PHE:HD1  | 1:33:A:LYS:H    | 13       | 1.39          |
| (1,1116) | 1:14:A:TYR:HD1  | 1:36:A:THR:HG21 | 12       | 1.38          |
| (1,1116) | 1:14:A:TYR:HD1  | 1:36:A:THR:HG22 | 12       | 1.38          |
| (1,1116) | 1:14:A:TYR:HD1  | 1:36:A:THR:HG23 | 12       | 1.38          |
| (1,848)  | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1  | 10       | 1.38          |
| (1,848)  | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1  | 13       | 1.38          |
| (1,134)  | 1:31:A:PHE:HD1  | 1:33:A:LYS:H    | 17       | 1.38          |
| (1,885)  | 1:16:A:VAL:HG11 | 1:31:A:PHE:HD1  | 19       | 1.37          |
| (1,885)  | 1:16:A:VAL:HG12 | 1:31:A:PHE:HD1  | 19       | 1.37          |
| (1,885)  | 1:16:A:VAL:HG13 | 1:31:A:PHE:HD1  | 19       | 1.37          |
| (1,848)  | 1:13:A:GLU:HA   | 1:14:A:TYR:HD1  | 7        | 1.37          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 4        | 1.37          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 15       | 1.37          |
| (1,848)  | 1:13:A:GLU:HA  | 1:14:A:TYR:HD1  | 15       | 1.36          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 8        | 1.36          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 10       | 1.36          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 7        | 1.35          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 7        | 1.35          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 7        | 1.35          |
| (1,848)  | 1:13:A:GLU:HA  | 1:14:A:TYR:HD1  | 17       | 1.35          |
| (1,848)  | 1:13:A:GLU:HA  | 1:14:A:TYR:HD1  | 18       | 1.35          |
| (1,848)  | 1:13:A:GLU:HA  | 1:14:A:TYR:HD1  | 19       | 1.35          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 1        | 1.35          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 5        | 1.35          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 7        | 1.35          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 12       | 1.35          |
| (1,848)  | 1:13:A:GLU:HA  | 1:14:A:TYR:HD1  | 1        | 1.34          |
| (1,848)  | 1:13:A:GLU:HA  | 1:14:A:TYR:HD1  | 4        | 1.34          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 9        | 1.34          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 11       | 1.34          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 14       | 1.34          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 3        | 1.33          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 2        | 1.32          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 14       | 1.31          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 16       | 1.31          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 18       | 1.31          |
| (1,134)  | 1:31:A:PHE:HD1 | 1:33:A:LYS:H    | 20       | 1.31          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 6        | 1.25          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 4        | 1.24          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 4        | 1.24          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 4        | 1.24          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 3        | 1.24          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 8        | 1.23          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 5        | 1.22          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 10       | 1.2           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 10       | 1.2           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 10       | 1.2           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 13       | 1.2           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 13       | 1.2           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 13       | 1.2           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 18       | 1.2           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 18       | 1.2           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 18       | 1.2           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 20       | 1.18          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 20       | 1.18          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 20       | 1.18          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 11       | 1.17          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 11       | 1.17          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 11       | 1.17          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 12       | 1.16          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 12       | 1.16          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 12       | 1.16          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 6        | 1.16          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 5        | 1.16          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 16       | 1.16          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 7        | 1.15          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 7        | 1.15          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 7        | 1.15          |
| (1,818)  | 1:9:A:TRP:HB3  | 1:14:A:TYR:HE1  | 16       | 1.14          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 8        | 1.14          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 14       | 1.14          |
| (1,799)  | 1:7:A:VAL:HB   | 1:14:A:TYR:HD1  | 9        | 1.12          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 15       | 1.11          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 15       | 1.11          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 15       | 1.11          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 12       | 1.11          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 20       | 1.11          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 17       | 1.1           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 17       | 1.09          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 17       | 1.09          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 17       | 1.09          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 2        | 1.09          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 3        | 1.09          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 7        | 1.09          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 13       | 1.09          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 4        | 1.08          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 19       | 1.07          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 19       | 1.07          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 19       | 1.07          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 1        | 1.07          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 9        | 1.07          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 11       | 1.07          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 18       | 1.07          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 19       | 1.07          |
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 10       | 1.06          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,303)  | 1:14:A:TYR:H   | 1:14:A:TYR:HE1  | 15       | 1.02          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 4        | 1.01          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 4        | 1.01          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 4        | 1.01          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 10       | 0.97          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 10       | 0.97          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 10       | 0.97          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 1        | 0.96          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 1        | 0.96          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 1        | 0.96          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 2        | 0.96          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 2        | 0.96          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 2        | 0.96          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 8        | 0.93          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 8        | 0.93          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 8        | 0.93          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 11       | 0.93          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 11       | 0.93          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 11       | 0.93          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 13       | 0.93          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 13       | 0.93          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 13       | 0.93          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 3        | 0.92          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 3        | 0.92          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 3        | 0.92          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 8        | 0.88          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 8        | 0.88          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 8        | 0.88          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 3        | 0.87          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 3        | 0.87          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 3        | 0.87          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 18       | 0.87          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 18       | 0.87          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 18       | 0.87          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 20       | 0.86          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 20       | 0.86          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 20       | 0.86          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 15       | 0.84          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 15       | 0.84          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 15       | 0.84          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 17       | 0.82          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 17       | 0.82          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 17       | 0.82          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 19       | 0.82          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 19       | 0.82          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 19       | 0.82          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 9        | 0.8           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 9        | 0.8           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 9        | 0.8           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 6        | 0.7           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 6        | 0.7           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 6        | 0.7           |
| (1,1125) | 1:33:A:LYS:HB2 | 1:38:A:VAL:HB   | 9        | 0.69          |
| (1,1125) | 1:33:A:LYS:HB2 | 1:38:A:VAL:HB   | 18       | 0.69          |
| (1,1125) | 1:33:A:LYS:HB2 | 1:38:A:VAL:HB   | 14       | 0.68          |
| (1,1125) | 1:33:A:LYS:HB2 | 1:38:A:VAL:HB   | 16       | 0.68          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 6        | 0.68          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 6        | 0.68          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 6        | 0.68          |
| (1,1125) | 1:33:A:LYS:HB2 | 1:38:A:VAL:HB   | 4        | 0.67          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 1        | 0.67          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 1        | 0.67          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 1        | 0.67          |
| (1,1125) | 1:33:A:LYS:HB2 | 1:38:A:VAL:HB   | 7        | 0.66          |
| (1,1125) | 1:33:A:LYS:HB2 | 1:38:A:VAL:HB   | 10       | 0.66          |
| (1,1125) | 1:33:A:LYS:HB2 | 1:38:A:VAL:HB   | 12       | 0.66          |
| (1,1125) | 1:33:A:LYS:HB2 | 1:38:A:VAL:HB   | 13       | 0.66          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 2        | 0.66          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 2        | 0.66          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 2        | 0.66          |
| (1,1125) | 1:33:A:LYS:HB2 | 1:38:A:VAL:HB   | 15       | 0.65          |
| (1,1125) | 1:33:A:LYS:HB2 | 1:38:A:VAL:HB   | 19       | 0.65          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 14       | 0.63          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 14       | 0.63          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 14       | 0.63          |
| (1,445)  | 1:43:A:GLN:H   | 1:43:A:GLN:HG3  | 11       | 0.63          |
| (1,287)  | 1:13:A:GLU:H   | 1:14:A:TYR:HE1  | 5        | 0.6           |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG21 | 5        | 0.59          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG22 | 5        | 0.59          |
| (1,1116) | 1:14:A:TYR:HD1 | 1:36:A:THR:HG23 | 5        | 0.59          |
| (1,287)  | 1:13:A:GLU:H   | 1:14:A:TYR:HE1  | 16       | 0.58          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG21 | 9        | 0.57          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG22 | 9        | 0.57          |
| (1,1115) | 1:14:A:TYR:HE1 | 1:36:A:THR:HG23 | 9        | 0.57          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,287)  | 1:13:A:GLU:H    | 1:14:A:TYR:HE1  | 6        | 0.55          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 9        | 0.53          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 9        | 0.53          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 9        | 0.53          |
| (1,1115) | 1:14:A:TYR:HE1  | 1:36:A:THR:HG21 | 5        | 0.52          |
| (1,1115) | 1:14:A:TYR:HE1  | 1:36:A:THR:HG22 | 5        | 0.52          |
| (1,1115) | 1:14:A:TYR:HE1  | 1:36:A:THR:HG23 | 5        | 0.52          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 3        | 0.47          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 3        | 0.47          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 3        | 0.47          |
| (1,287)  | 1:13:A:GLU:H    | 1:14:A:TYR:HE1  | 3        | 0.46          |
| (1,288)  | 1:13:A:GLU:H    | 1:14:A:TYR:HD1  | 5        | 0.45          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O    | 1        | 0.44          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O    | 19       | 0.44          |
| (1,1115) | 1:14:A:TYR:HE1  | 1:36:A:THR:HG21 | 14       | 0.44          |
| (1,1115) | 1:14:A:TYR:HE1  | 1:36:A:THR:HG22 | 14       | 0.44          |
| (1,1115) | 1:14:A:TYR:HE1  | 1:36:A:THR:HG23 | 14       | 0.44          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 18       | 0.44          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 18       | 0.44          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 18       | 0.44          |
| (1,288)  | 1:13:A:GLU:H    | 1:14:A:TYR:HD1  | 16       | 0.44          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O    | 2        | 0.43          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O    | 5        | 0.43          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O    | 6        | 0.43          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O    | 11       | 0.43          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O    | 17       | 0.42          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 8        | 0.42          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 8        | 0.42          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 8        | 0.42          |
| (1,844)  | 1:12:A:GLN:HG2  | 1:14:A:TYR:HE1  | 6        | 0.42          |
| (1,844)  | 1:12:A:GLN:HG3  | 1:14:A:TYR:HE1  | 6        | 0.42          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD2  | 1        | 0.42          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD3  | 1        | 0.42          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O    | 3        | 0.41          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O    | 8        | 0.41          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O    | 13       | 0.41          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O    | 15       | 0.41          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H    | 7        | 0.4           |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H    | 12       | 0.4           |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG2  | 20       | 0.4           |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG3  | 20       | 0.4           |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD2  | 17       | 0.4           |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD3 | 17       | 0.4           |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 4        | 0.39          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O   | 10       | 0.39          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB2 | 7        | 0.39          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB3 | 7        | 0.39          |
| (1,288)  | 1:13:A:GLU:H    | 1:14:A:TYR:HD1 | 6        | 0.39          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 10       | 0.38          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 13       | 0.38          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 19       | 0.38          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 11       | 0.37          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 15       | 0.37          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O   | 7        | 0.37          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O   | 12       | 0.37          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O   | 16       | 0.37          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB2 | 12       | 0.37          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB3 | 12       | 0.37          |
| (1,1121) | 1:38:A:VAL:HA   | 1:78:A:ARG:HD2 | 5        | 0.37          |
| (1,1121) | 1:38:A:VAL:HA   | 1:78:A:ARG:HD3 | 5        | 0.37          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 2        | 0.36          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 14       | 0.36          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 16       | 0.36          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O   | 4        | 0.36          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB2 | 4        | 0.36          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB3 | 4        | 0.36          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB2 | 14       | 0.36          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB3 | 14       | 0.36          |
| (1,1121) | 1:38:A:VAL:HA   | 1:78:A:ARG:HD2 | 8        | 0.36          |
| (1,1121) | 1:38:A:VAL:HA   | 1:78:A:ARG:HD3 | 8        | 0.36          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1 | 5        | 0.36          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1 | 5        | 0.36          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1 | 5        | 0.36          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1 | 20       | 0.36          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1 | 20       | 0.36          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1 | 20       | 0.36          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 6        | 0.35          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB  | 6        | 0.35          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB  | 6        | 0.35          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB2 | 13       | 0.35          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB3 | 13       | 0.35          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB2 | 19       | 0.35          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB3 | 19       | 0.35          |
| (1,287)  | 1:13:A:GLU:H    | 1:14:A:TYR:HE1 | 14       | 0.35          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 3        | 0.34          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 8        | 0.34          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 18       | 0.34          |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG2 | 3        | 0.34          |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG3 | 3        | 0.34          |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA2 | 20       | 0.34          |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA3 | 20       | 0.34          |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA2 | 20       | 0.34          |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA3 | 20       | 0.34          |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA2 | 20       | 0.34          |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA3 | 20       | 0.34          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB2 | 10       | 0.34          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB3 | 10       | 0.34          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB2 | 15       | 0.34          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB3 | 15       | 0.34          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB2 | 16       | 0.34          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB3 | 16       | 0.34          |
| (1,287)  | 1:13:A:GLU:H    | 1:14:A:TYR:HE1 | 9        | 0.34          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 1        | 0.33          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 9        | 0.33          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 20       | 0.33          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O   | 14       | 0.33          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1 | 6        | 0.33          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1 | 6        | 0.33          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1 | 6        | 0.33          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 5        | 0.32          |
| (2,25)   | 1:31:A:PHE:O    | 1:35:A:LEU:H   | 17       | 0.32          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB  | 20       | 0.32          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB  | 20       | 0.32          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA  | 14       | 0.32          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA  | 14       | 0.32          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA  | 14       | 0.32          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1 | 14       | 0.32          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1 | 14       | 0.32          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1 | 14       | 0.32          |
| (1,287)  | 1:13:A:GLU:H    | 1:14:A:TYR:HE1 | 13       | 0.32          |
| (2,17)   | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 17       | 0.31          |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG2 | 2        | 0.31          |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG3 | 2        | 0.31          |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG2 | 11       | 0.31          |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG3 | 11       | 0.31          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA  | 7        | 0.31          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,988) | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA  | 7        | 0.31          |
| (1,988) | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA  | 7        | 0.31          |
| (1,988) | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA  | 8        | 0.31          |
| (1,988) | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA  | 8        | 0.31          |
| (1,988) | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA  | 8        | 0.31          |
| (1,970) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA  | 3        | 0.31          |
| (1,970) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA  | 3        | 0.31          |
| (1,970) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA  | 3        | 0.31          |
| (1,970) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA  | 5        | 0.31          |
| (1,970) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA  | 5        | 0.31          |
| (1,970) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA  | 5        | 0.31          |
| (1,288) | 1:13:A:GLU:H    | 1:14:A:TYR:HD1 | 3        | 0.31          |
| (1,876) | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1 | 16       | 0.3           |
| (1,876) | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1 | 16       | 0.3           |
| (1,876) | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1 | 16       | 0.3           |
| (1,844) | 1:12:A:GLN:HG2  | 1:14:A:TYR:HE1 | 17       | 0.3           |
| (1,844) | 1:12:A:GLN:HG3  | 1:14:A:TYR:HE1 | 17       | 0.3           |
| (2,17)  | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 10       | 0.29          |
| (1,988) | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA  | 3        | 0.29          |
| (1,988) | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA  | 3        | 0.29          |
| (1,988) | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA  | 3        | 0.29          |
| (1,988) | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA  | 12       | 0.29          |
| (1,988) | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA  | 12       | 0.29          |
| (1,988) | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA  | 12       | 0.29          |
| (1,988) | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA  | 13       | 0.29          |
| (1,988) | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA  | 13       | 0.29          |
| (1,988) | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA  | 13       | 0.29          |
| (1,988) | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA  | 16       | 0.29          |
| (1,988) | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA  | 16       | 0.29          |
| (1,988) | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA  | 16       | 0.29          |
| (1,876) | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1 | 12       | 0.29          |
| (1,876) | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1 | 12       | 0.29          |
| (1,876) | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1 | 12       | 0.29          |
| (1,844) | 1:12:A:GLN:HG2  | 1:14:A:TYR:HE1 | 7        | 0.29          |
| (1,844) | 1:12:A:GLN:HG3  | 1:14:A:TYR:HE1 | 7        | 0.29          |
| (2,17)  | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 2        | 0.28          |
| (2,17)  | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 4        | 0.28          |
| (2,17)  | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 7        | 0.28          |
| (2,17)  | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 12       | 0.28          |
| (2,17)  | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 13       | 0.28          |
| (2,17)  | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 16       | 0.28          |
| (2,17)  | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 19       | 0.28          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB  | 1        | 0.28          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB  | 1        | 0.28          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA  | 4        | 0.28          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA  | 4        | 0.28          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA  | 4        | 0.28          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA  | 16       | 0.28          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA  | 16       | 0.28          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA  | 16       | 0.28          |
| (2,17)   | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 11       | 0.27          |
| (2,17)   | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 14       | 0.27          |
| (2,17)   | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 18       | 0.27          |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG2 | 6        | 0.27          |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG3 | 6        | 0.27          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA  | 9        | 0.27          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA  | 9        | 0.27          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA  | 9        | 0.27          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA  | 9        | 0.27          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA  | 9        | 0.27          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA  | 9        | 0.27          |
| (1,1436) | 1:77:A:THR:HB   | 1:78:A:ARG:HD2 | 1        | 0.27          |
| (1,1436) | 1:77:A:THR:HB   | 1:78:A:ARG:HD3 | 1        | 0.27          |
| (1,1131) | 1:38:A:VAL:HG21 | 1:74:A:MET:HB3 | 18       | 0.27          |
| (1,1131) | 1:38:A:VAL:HG22 | 1:74:A:MET:HB3 | 18       | 0.27          |
| (1,1131) | 1:38:A:VAL:HG23 | 1:74:A:MET:HB3 | 18       | 0.27          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA  | 5        | 0.27          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA  | 5        | 0.27          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA  | 5        | 0.27          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA  | 9        | 0.27          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA  | 9        | 0.27          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA  | 9        | 0.27          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA  | 11       | 0.27          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA  | 11       | 0.27          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA  | 11       | 0.27          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA  | 9        | 0.27          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA  | 9        | 0.27          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA  | 9        | 0.27          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA  | 18       | 0.27          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA  | 18       | 0.27          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA  | 18       | 0.27          |
| (1,287)  | 1:13:A:GLU:H    | 1:14:A:TYR:HE1 | 17       | 0.27          |
| (2,17)   | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 1        | 0.26          |
| (2,17)   | 1:27:A:ASP:O    | 1:31:A:PHE:H   | 3        | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,17)   | 1:27:A:ASP:O    | 1:31:A:PHE:H    | 5        | 0.26          |
| (2,17)   | 1:27:A:ASP:O    | 1:31:A:PHE:H    | 8        | 0.26          |
| (2,17)   | 1:27:A:ASP:O    | 1:31:A:PHE:H    | 15       | 0.26          |
| (2,17)   | 1:27:A:ASP:O    | 1:31:A:PHE:H    | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG11 | 1:77:A:THR:HG21 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG11 | 1:77:A:THR:HG22 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG11 | 1:77:A:THR:HG23 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG12 | 1:77:A:THR:HG21 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG12 | 1:77:A:THR:HG22 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG12 | 1:77:A:THR:HG23 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG13 | 1:77:A:THR:HG21 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG13 | 1:77:A:THR:HG22 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG13 | 1:77:A:THR:HG23 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG21 | 1:77:A:THR:HG21 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG21 | 1:77:A:THR:HG22 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG21 | 1:77:A:THR:HG23 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG22 | 1:77:A:THR:HG21 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG22 | 1:77:A:THR:HG22 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG22 | 1:77:A:THR:HG23 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG23 | 1:77:A:THR:HG21 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG23 | 1:77:A:THR:HG22 | 20       | 0.26          |
| (1,1702) | 1:38:A:VAL:HG23 | 1:77:A:THR:HG23 | 20       | 0.26          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA   | 6        | 0.26          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA   | 6        | 0.26          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA   | 6        | 0.26          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA   | 10       | 0.26          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA   | 10       | 0.26          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA   | 10       | 0.26          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA   | 14       | 0.26          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA   | 14       | 0.26          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA   | 14       | 0.26          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA   | 15       | 0.26          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA   | 15       | 0.26          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA   | 15       | 0.26          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA   | 18       | 0.26          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA   | 18       | 0.26          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA   | 18       | 0.26          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O    | 2        | 0.25          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O    | 6        | 0.25          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG11 | 12       | 0.25          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG12 | 12       | 0.25          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG13 | 12       | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG21 | 12       | 0.25          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG22 | 12       | 0.25          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG23 | 12       | 0.25          |
| (1,1722) | 1:44:A:LYS:HG2  | 1:45:A:LEU:H    | 18       | 0.25          |
| (1,1722) | 1:44:A:LYS:HG3  | 1:45:A:LEU:H    | 18       | 0.25          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA   | 18       | 0.25          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA   | 18       | 0.25          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 18       | 0.25          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 18       | 0.25          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 18       | 0.25          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 18       | 0.25          |
| (1,1436) | 1:77:A:THR:HB   | 1:78:A:ARG:HD2  | 17       | 0.25          |
| (1,1436) | 1:77:A:THR:HB   | 1:78:A:ARG:HD3  | 17       | 0.25          |
| (1,1131) | 1:38:A:VAL:HG21 | 1:74:A:MET:HB3  | 9        | 0.25          |
| (1,1131) | 1:38:A:VAL:HG22 | 1:74:A:MET:HB3  | 9        | 0.25          |
| (1,1131) | 1:38:A:VAL:HG23 | 1:74:A:MET:HB3  | 9        | 0.25          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA   | 1        | 0.25          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA   | 1        | 0.25          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA   | 1        | 0.25          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA   | 2        | 0.25          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA   | 2        | 0.25          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA   | 2        | 0.25          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA   | 17       | 0.25          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA   | 17       | 0.25          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA   | 17       | 0.25          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA   | 19       | 0.25          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA   | 19       | 0.25          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA   | 19       | 0.25          |
| (1,988)  | 1:26:A:LEU:HD11 | 1:58:A:ASP:HA   | 20       | 0.25          |
| (1,988)  | 1:26:A:LEU:HD12 | 1:58:A:ASP:HA   | 20       | 0.25          |
| (1,988)  | 1:26:A:LEU:HD13 | 1:58:A:ASP:HA   | 20       | 0.25          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 7        | 0.25          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 7        | 0.25          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 7        | 0.25          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 11       | 0.25          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 11       | 0.25          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 11       | 0.25          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 3        | 0.25          |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 3        | 0.25          |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 3        | 0.25          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 13       | 0.25          |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 13       | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 13       | 0.25          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 20       | 0.25          |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 20       | 0.25          |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 20       | 0.25          |
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 8        | 0.25          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD2  | 8        | 0.25          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD3  | 8        | 0.25          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O    | 1        | 0.24          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O    | 11       | 0.24          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O    | 19       | 0.24          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG11 | 20       | 0.24          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG12 | 20       | 0.24          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG13 | 20       | 0.24          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG21 | 20       | 0.24          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG22 | 20       | 0.24          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG23 | 20       | 0.24          |
| (1,1407) | 1:73:A:MET:HB2  | 1:74:A:MET:HG3  | 17       | 0.24          |
| (1,1407) | 1:73:A:MET:HB3  | 1:74:A:MET:HG3  | 17       | 0.24          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA   | 17       | 0.24          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA   | 17       | 0.24          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA   | 17       | 0.24          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 1        | 0.24          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 1        | 0.24          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 1        | 0.24          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 2        | 0.24          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 2        | 0.24          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 2        | 0.24          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 15       | 0.24          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 15       | 0.24          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 15       | 0.24          |
| (1,844)  | 1:12:A:GLN:HG2  | 1:14:A:TYR:HE1  | 13       | 0.24          |
| (1,844)  | 1:12:A:GLN:HG3  | 1:14:A:TYR:HE1  | 13       | 0.24          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 4        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 4        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 4        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 5        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 5        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 5        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 6        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 6        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 6        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 7        | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 7        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 7        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 8        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 8        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 8        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 9        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 9        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 9        | 0.24          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 10       | 0.24          |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 10       | 0.24          |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 10       | 0.24          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 12       | 0.24          |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 12       | 0.24          |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 12       | 0.24          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 17       | 0.24          |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 17       | 0.24          |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 17       | 0.24          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 19       | 0.24          |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 19       | 0.24          |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 19       | 0.24          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 5        | 0.24          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 5        | 0.24          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 8        | 0.24          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 8        | 0.24          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 13       | 0.24          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 13       | 0.24          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD2  | 5        | 0.24          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD3  | 5        | 0.24          |
| (2,17)   | 1:27:A:ASP:O    | 1:31:A:PHE:H    | 6        | 0.23          |
| (2,17)   | 1:27:A:ASP:O    | 1:31:A:PHE:H    | 9        | 0.23          |
| (1,1843) | 1:64:A:LEU:HA   | 1:65:A:LYS:HE2  | 15       | 0.23          |
| (1,1843) | 1:64:A:LEU:HA   | 1:65:A:LYS:HE3  | 15       | 0.23          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG11 | 8        | 0.23          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG12 | 8        | 0.23          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG13 | 8        | 0.23          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG21 | 8        | 0.23          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG22 | 8        | 0.23          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG23 | 8        | 0.23          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB   | 17       | 0.23          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB   | 17       | 0.23          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 4        | 0.23          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 4        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 4        | 0.23          |
| (1,844)  | 1:12:A:GLN:HG2  | 1:14:A:TYR:HE1  | 8        | 0.23          |
| (1,844)  | 1:12:A:GLN:HG3  | 1:14:A:TYR:HE1  | 8        | 0.23          |
| (1,844)  | 1:12:A:GLN:HG2  | 1:14:A:TYR:HE1  | 16       | 0.23          |
| (1,844)  | 1:12:A:GLN:HG3  | 1:14:A:TYR:HE1  | 16       | 0.23          |
| (1,844)  | 1:12:A:GLN:HG2  | 1:14:A:TYR:HE1  | 19       | 0.23          |
| (1,844)  | 1:12:A:GLN:HG3  | 1:14:A:TYR:HE1  | 19       | 0.23          |
| (1,772)  | 1:6:A:ILE:HG21  | 1:71:A:LYS:HG2  | 1        | 0.23          |
| (1,772)  | 1:6:A:ILE:HG22  | 1:71:A:LYS:HG2  | 1        | 0.23          |
| (1,772)  | 1:6:A:ILE:HG23  | 1:71:A:LYS:HG2  | 1        | 0.23          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 2        | 0.23          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 2        | 0.23          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 7        | 0.23          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 7        | 0.23          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 16       | 0.23          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 16       | 0.23          |
| (1,288)  | 1:13:A:GLU:H    | 1:14:A:TYR:HD1  | 13       | 0.23          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O    | 5        | 0.22          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG11 | 3        | 0.22          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG12 | 3        | 0.22          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG13 | 3        | 0.22          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG21 | 3        | 0.22          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG22 | 3        | 0.22          |
| (1,1810) | 1:57:A:ASN:H    | 1:59:A:VAL:HG23 | 3        | 0.22          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB   | 7        | 0.22          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB   | 7        | 0.22          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB   | 13       | 0.22          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB   | 13       | 0.22          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA   | 5        | 0.22          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA   | 5        | 0.22          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 5        | 0.22          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 5        | 0.22          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 5        | 0.22          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 5        | 0.22          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA   | 20       | 0.22          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA   | 20       | 0.22          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 20       | 0.22          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 20       | 0.22          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 20       | 0.22          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 20       | 0.22          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 6        | 0.22          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 6        | 0.22          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2 | 6        | 0.22          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3 | 6        | 0.22          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2 | 6        | 0.22          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3 | 6        | 0.22          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2 | 12       | 0.22          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3 | 12       | 0.22          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2 | 12       | 0.22          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3 | 12       | 0.22          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2 | 12       | 0.22          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3 | 12       | 0.22          |
| (1,844)  | 1:12:A:GLN:HG2  | 1:14:A:TYR:HE1 | 10       | 0.22          |
| (1,844)  | 1:12:A:GLN:HG3  | 1:14:A:TYR:HE1 | 10       | 0.22          |
| (1,288)  | 1:13:A:GLU:H    | 1:14:A:TYR:HD1 | 9        | 0.22          |
| (1,288)  | 1:13:A:GLU:H    | 1:14:A:TYR:HD1 | 14       | 0.22          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD2 | 13       | 0.22          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD3 | 13       | 0.22          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O   | 3        | 0.21          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O   | 8        | 0.21          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O   | 15       | 0.21          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O   | 17       | 0.21          |
| (2,9)    | 1:44:A:LYS:H    | 1:75:A:MET:O   | 20       | 0.21          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB  | 4        | 0.21          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB  | 4        | 0.21          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB  | 10       | 0.21          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB  | 10       | 0.21          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB  | 12       | 0.21          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB  | 12       | 0.21          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB  | 15       | 0.21          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB  | 15       | 0.21          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB  | 19       | 0.21          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB  | 19       | 0.21          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA  | 16       | 0.21          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA  | 16       | 0.21          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA  | 16       | 0.21          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA  | 16       | 0.21          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA  | 16       | 0.21          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA  | 16       | 0.21          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2 | 13       | 0.21          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3 | 13       | 0.21          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2 | 13       | 0.21          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3 | 13       | 0.21          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2 | 13       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 13       | 0.21          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 15       | 0.21          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 15       | 0.21          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 15       | 0.21          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 15       | 0.21          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 15       | 0.21          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 15       | 0.21          |
| (1,1407) | 1:73:A:MET:HB2  | 1:74:A:MET:HG3  | 16       | 0.21          |
| (1,1407) | 1:73:A:MET:HB3  | 1:74:A:MET:HG3  | 16       | 0.21          |
| (1,1116) | 1:14:A:TYR:HD1  | 1:36:A:THR:HG21 | 16       | 0.21          |
| (1,1116) | 1:14:A:TYR:HD1  | 1:36:A:THR:HG22 | 16       | 0.21          |
| (1,1116) | 1:14:A:TYR:HD1  | 1:36:A:THR:HG23 | 16       | 0.21          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA   | 6        | 0.21          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA   | 6        | 0.21          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA   | 6        | 0.21          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA   | 8        | 0.21          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA   | 8        | 0.21          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA   | 8        | 0.21          |
| (1,454)  | 1:29:A:LYS:HE2  | 1:45:A:LEU:H    | 18       | 0.21          |
| (1,288)  | 1:13:A:GLU:H    | 1:14:A:TYR:HD1  | 17       | 0.21          |
| (1,232)  | 1:38:A:VAL:HB   | 1:79:A:GLU:H    | 5        | 0.21          |
| (1,232)  | 1:38:A:VAL:HB   | 1:79:A:GLU:H    | 8        | 0.21          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD2  | 15       | 0.21          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD3  | 15       | 0.21          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O    | 13       | 0.2           |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA   | 3        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA   | 3        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 3        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 3        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 3        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 3        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA   | 6        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA   | 6        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 6        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 6        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 6        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 6        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA   | 8        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA   | 8        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 8        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 8        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 8        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 8        | 0.2           |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA   | 14       | 0.2           |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA   | 14       | 0.2           |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 14       | 0.2           |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 14       | 0.2           |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 14       | 0.2           |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 14       | 0.2           |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 1        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 1        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 1        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 1        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 1        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 1        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 4        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 4        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 4        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 4        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 4        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 4        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 8        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 8        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 8        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 8        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 8        | 0.2           |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 8        | 0.2           |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 1        | 0.2           |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA   | 11       | 0.2           |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA   | 11       | 0.2           |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA   | 11       | 0.2           |
| (1,844)  | 1:12:A:GLN:HG2  | 1:14:A:TYR:HE1  | 20       | 0.2           |
| (1,844)  | 1:12:A:GLN:HG3  | 1:14:A:TYR:HE1  | 20       | 0.2           |
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 10       | 0.2           |
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 15       | 0.2           |
| (1,447)  | 1:43:A:GLN:H    | 1:43:A:GLN:HG2  | 6        | 0.2           |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD2  | 10       | 0.2           |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD3  | 10       | 0.2           |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O    | 10       | 0.19          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB   | 8        | 0.19          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB   | 8        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG11 | 1:77:A:THR:HG21 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG11 | 1:77:A:THR:HG22 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG11 | 1:77:A:THR:HG23 | 6        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1702) | 1:38:A:VAL:HG12 | 1:77:A:THR:HG21 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG12 | 1:77:A:THR:HG22 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG12 | 1:77:A:THR:HG23 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG13 | 1:77:A:THR:HG21 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG13 | 1:77:A:THR:HG22 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG13 | 1:77:A:THR:HG23 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG21 | 1:77:A:THR:HG21 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG21 | 1:77:A:THR:HG22 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG21 | 1:77:A:THR:HG23 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG22 | 1:77:A:THR:HG21 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG22 | 1:77:A:THR:HG22 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG22 | 1:77:A:THR:HG23 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG23 | 1:77:A:THR:HG21 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG23 | 1:77:A:THR:HG22 | 6        | 0.19          |
| (1,1702) | 1:38:A:VAL:HG23 | 1:77:A:THR:HG23 | 6        | 0.19          |
| (1,1687) | 1:38:A:VAL:HG11 | 1:40:A:PRO:HA   | 20       | 0.19          |
| (1,1687) | 1:38:A:VAL:HG12 | 1:40:A:PRO:HA   | 20       | 0.19          |
| (1,1687) | 1:38:A:VAL:HG13 | 1:40:A:PRO:HA   | 20       | 0.19          |
| (1,1687) | 1:38:A:VAL:HG21 | 1:40:A:PRO:HA   | 20       | 0.19          |
| (1,1687) | 1:38:A:VAL:HG22 | 1:40:A:PRO:HA   | 20       | 0.19          |
| (1,1687) | 1:38:A:VAL:HG23 | 1:40:A:PRO:HA   | 20       | 0.19          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 10       | 0.19          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 10       | 0.19          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 10       | 0.19          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 10       | 0.19          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 10       | 0.19          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 10       | 0.19          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 20       | 0.19          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 20       | 0.19          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 20       | 0.19          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 20       | 0.19          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 20       | 0.19          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 20       | 0.19          |
| (1,1407) | 1:73:A:MET:HB2  | 1:74:A:MET:HG3  | 3        | 0.19          |
| (1,1407) | 1:73:A:MET:HB3  | 1:74:A:MET:HG3  | 3        | 0.19          |
| (1,1407) | 1:73:A:MET:HB2  | 1:74:A:MET:HG3  | 19       | 0.19          |
| (1,1407) | 1:73:A:MET:HB3  | 1:74:A:MET:HG3  | 19       | 0.19          |
| (1,1175) | 1:43:A:GLN:HG3  | 1:77:A:THR:HG21 | 6        | 0.19          |
| (1,1175) | 1:43:A:GLN:HG3  | 1:77:A:THR:HG22 | 6        | 0.19          |
| (1,1175) | 1:43:A:GLN:HG3  | 1:77:A:THR:HG23 | 6        | 0.19          |
| (1,1127) | 1:33:A:LYS:HD3  | 1:38:A:VAL:HB   | 13       | 0.19          |
| (1,1121) | 1:38:A:VAL:HA   | 1:78:A:ARG:HD2  | 11       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1121) | 1:38:A:VAL:HA   | 1:78:A:ARG:HD3  | 11       | 0.19          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 17       | 0.19          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD11 | 20       | 0.19          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD12 | 20       | 0.19          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD13 | 20       | 0.19          |
| (1,972)  | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 18       | 0.19          |
| (1,972)  | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 18       | 0.19          |
| (1,972)  | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 18       | 0.19          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA   | 4        | 0.19          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA   | 4        | 0.19          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA   | 4        | 0.19          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA   | 10       | 0.19          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA   | 10       | 0.19          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA   | 10       | 0.19          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA   | 15       | 0.19          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA   | 15       | 0.19          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA   | 15       | 0.19          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA   | 19       | 0.19          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA   | 19       | 0.19          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA   | 19       | 0.19          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 19       | 0.19          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 19       | 0.19          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 19       | 0.19          |
| (1,744)  | 1:2:A:ALA:HA    | 1:3:A:LEU:HG    | 13       | 0.19          |
| (1,655)  | 1:74:A:MET:HA   | 1:76:A:GLY:H    | 17       | 0.19          |
| (1,645)  | 1:44:A:LYS:H    | 1:75:A:MET:H    | 6        | 0.19          |
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 17       | 0.19          |
| (1,232)  | 1:38:A:VAL:HB   | 1:79:A:GLU:H    | 11       | 0.19          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD2  | 16       | 0.19          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD3  | 16       | 0.19          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 7        | 0.18          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB   | 5        | 0.18          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB   | 5        | 0.18          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA   | 1        | 0.18          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA   | 1        | 0.18          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 1        | 0.18          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 1        | 0.18          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 1        | 0.18          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 1        | 0.18          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA   | 7        | 0.18          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA   | 7        | 0.18          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 7        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 7        | 0.18          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 7        | 0.18          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 7        | 0.18          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA   | 11       | 0.18          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA   | 11       | 0.18          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 11       | 0.18          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 11       | 0.18          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 11       | 0.18          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 11       | 0.18          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA   | 17       | 0.18          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA   | 17       | 0.18          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 17       | 0.18          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 17       | 0.18          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 17       | 0.18          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 17       | 0.18          |
| (1,1551) | 1:9:A:TRP:HA    | 1:45:A:LEU:HD11 | 5        | 0.18          |
| (1,1551) | 1:9:A:TRP:HA    | 1:45:A:LEU:HD12 | 5        | 0.18          |
| (1,1551) | 1:9:A:TRP:HA    | 1:45:A:LEU:HD13 | 5        | 0.18          |
| (1,1551) | 1:9:A:TRP:HA    | 1:45:A:LEU:HD21 | 5        | 0.18          |
| (1,1551) | 1:9:A:TRP:HA    | 1:45:A:LEU:HD22 | 5        | 0.18          |
| (1,1551) | 1:9:A:TRP:HA    | 1:45:A:LEU:HD23 | 5        | 0.18          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 7        | 0.18          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 7        | 0.18          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 7        | 0.18          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 7        | 0.18          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 7        | 0.18          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 7        | 0.18          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 11       | 0.18          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 11       | 0.18          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 11       | 0.18          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 11       | 0.18          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 11       | 0.18          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 11       | 0.18          |
| (1,1264) | 1:59:A:VAL:HA   | 1:64:A:LEU:HG   | 8        | 0.18          |
| (1,1127) | 1:33:A:LYS:HD3  | 1:38:A:VAL:HB   | 15       | 0.18          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 15       | 0.18          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD11 | 9        | 0.18          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD12 | 9        | 0.18          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD13 | 9        | 0.18          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA   | 1        | 0.18          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA   | 1        | 0.18          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA   | 1        | 0.18          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA  | 2        | 0.18          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA  | 2        | 0.18          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA  | 2        | 0.18          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA  | 12       | 0.18          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA  | 12       | 0.18          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA  | 12       | 0.18          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA  | 13       | 0.18          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA  | 13       | 0.18          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA  | 13       | 0.18          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1 | 10       | 0.18          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1 | 10       | 0.18          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1 | 10       | 0.18          |
| (1,844)  | 1:12:A:GLN:HG2  | 1:14:A:TYR:HE1 | 4        | 0.18          |
| (1,844)  | 1:12:A:GLN:HG3  | 1:14:A:TYR:HE1 | 4        | 0.18          |
| (1,655)  | 1:74:A:MET:HA   | 1:76:A:GLY:H   | 5        | 0.18          |
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H   | 14       | 0.18          |
| (1,252)  | 1:7:A:VAL:H     | 1:32:A:LEU:HB2 | 8        | 0.18          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD2 | 19       | 0.18          |
| (1,188)  | 1:38:A:VAL:H    | 1:78:A:ARG:HD3 | 19       | 0.18          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N   | 4        | 0.17          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N   | 12       | 0.17          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O   | 7        | 0.17          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O   | 16       | 0.17          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB  | 2        | 0.17          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB  | 2        | 0.17          |
| (1,1698) | 1:38:A:VAL:HG11 | 1:76:A:GLY:H   | 18       | 0.17          |
| (1,1698) | 1:38:A:VAL:HG12 | 1:76:A:GLY:H   | 18       | 0.17          |
| (1,1698) | 1:38:A:VAL:HG13 | 1:76:A:GLY:H   | 18       | 0.17          |
| (1,1698) | 1:38:A:VAL:HG21 | 1:76:A:GLY:H   | 18       | 0.17          |
| (1,1698) | 1:38:A:VAL:HG22 | 1:76:A:GLY:H   | 18       | 0.17          |
| (1,1698) | 1:38:A:VAL:HG23 | 1:76:A:GLY:H   | 18       | 0.17          |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG2 | 17       | 0.17          |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG3 | 17       | 0.17          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA  | 2        | 0.17          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA  | 2        | 0.17          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA  | 2        | 0.17          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA  | 2        | 0.17          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA  | 2        | 0.17          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA  | 2        | 0.17          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA  | 4        | 0.17          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA  | 4        | 0.17          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA  | 4        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 4        | 0.17          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 4        | 0.17          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 4        | 0.17          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA   | 19       | 0.17          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA   | 19       | 0.17          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 19       | 0.17          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 19       | 0.17          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 19       | 0.17          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 19       | 0.17          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 2        | 0.17          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 2        | 0.17          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 2        | 0.17          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 2        | 0.17          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 2        | 0.17          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 2        | 0.17          |
| (1,1407) | 1:73:A:MET:HB2  | 1:74:A:MET:HG3  | 14       | 0.17          |
| (1,1407) | 1:73:A:MET:HB3  | 1:74:A:MET:HG3  | 14       | 0.17          |
| (1,1317) | 1:61:A:LEU:HA   | 1:64:A:LEU:HG   | 15       | 0.17          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 18       | 0.17          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 18       | 0.17          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 18       | 0.17          |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA2  | 17       | 0.17          |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA3  | 17       | 0.17          |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA2  | 17       | 0.17          |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA3  | 17       | 0.17          |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA2  | 17       | 0.17          |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA3  | 17       | 0.17          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 9        | 0.17          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 12       | 0.17          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 13       | 0.17          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD11 | 18       | 0.17          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD12 | 18       | 0.17          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD13 | 18       | 0.17          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA   | 7        | 0.17          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA   | 7        | 0.17          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA   | 7        | 0.17          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 13       | 0.17          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 13       | 0.17          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 13       | 0.17          |
| (1,744)  | 1:2:A:ALA:HA    | 1:3:A:LEU:HG    | 1        | 0.17          |
| (1,744)  | 1:2:A:ALA:HA    | 1:3:A:LEU:HG    | 18       | 0.17          |
| (1,655)  | 1:74:A:MET:HA   | 1:76:A:GLY:H    | 3        | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,655)  | 1:74:A:MET:HA   | 1:76:A:GLY:H   | 18       | 0.17          |
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H   | 1        | 0.17          |
| (1,252)  | 1:7:A:VAL:H     | 1:32:A:LEU:HB2 | 9        | 0.17          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N   | 10       | 0.16          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O   | 4        | 0.16          |
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O   | 12       | 0.16          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB  | 16       | 0.16          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB  | 16       | 0.16          |
| (1,1698) | 1:38:A:VAL:HG11 | 1:76:A:GLY:H   | 9        | 0.16          |
| (1,1698) | 1:38:A:VAL:HG12 | 1:76:A:GLY:H   | 9        | 0.16          |
| (1,1698) | 1:38:A:VAL:HG13 | 1:76:A:GLY:H   | 9        | 0.16          |
| (1,1698) | 1:38:A:VAL:HG21 | 1:76:A:GLY:H   | 9        | 0.16          |
| (1,1698) | 1:38:A:VAL:HG22 | 1:76:A:GLY:H   | 9        | 0.16          |
| (1,1698) | 1:38:A:VAL:HG23 | 1:76:A:GLY:H   | 9        | 0.16          |
| (1,1696) | 1:38:A:VAL:HG11 | 1:74:A:MET:HB3 | 20       | 0.16          |
| (1,1696) | 1:38:A:VAL:HG12 | 1:74:A:MET:HB3 | 20       | 0.16          |
| (1,1696) | 1:38:A:VAL:HG13 | 1:74:A:MET:HB3 | 20       | 0.16          |
| (1,1696) | 1:38:A:VAL:HG21 | 1:74:A:MET:HB3 | 20       | 0.16          |
| (1,1696) | 1:38:A:VAL:HG22 | 1:74:A:MET:HB3 | 20       | 0.16          |
| (1,1696) | 1:38:A:VAL:HG23 | 1:74:A:MET:HB3 | 20       | 0.16          |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG2 | 1        | 0.16          |
| (1,1681) | 1:38:A:VAL:H    | 1:78:A:ARG:HG3 | 1        | 0.16          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA  | 10       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA  | 10       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA  | 10       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA  | 10       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA  | 10       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA  | 10       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA  | 12       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA  | 12       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA  | 12       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA  | 12       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA  | 12       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA  | 12       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA  | 13       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA  | 13       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA  | 13       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA  | 13       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA  | 13       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA  | 13       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD11 | 1:30:A:GLN:HA  | 15       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD12 | 1:30:A:GLN:HA  | 15       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1635) | 1:26:A:LEU:HD13 | 1:30:A:GLN:HA   | 15       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD21 | 1:30:A:GLN:HA   | 15       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD22 | 1:30:A:GLN:HA   | 15       | 0.16          |
| (1,1635) | 1:26:A:LEU:HD23 | 1:30:A:GLN:HA   | 15       | 0.16          |
| (1,1549) | 1:8:A:LYS:HE2   | 1:9:A:TRP:H     | 1        | 0.16          |
| (1,1549) | 1:8:A:LYS:HE3   | 1:9:A:TRP:H     | 1        | 0.16          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 19       | 0.16          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 19       | 0.16          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 19       | 0.16          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 19       | 0.16          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 19       | 0.16          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 19       | 0.16          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG21 | 14       | 0.16          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG22 | 14       | 0.16          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG23 | 14       | 0.16          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG21 | 14       | 0.16          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG22 | 14       | 0.16          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG23 | 14       | 0.16          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG21 | 14       | 0.16          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG22 | 14       | 0.16          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG23 | 14       | 0.16          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 9        | 0.16          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 9        | 0.16          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 9        | 0.16          |
| (1,1135) | 1:33:A:LYS:HD2  | 1:38:A:VAL:HG11 | 17       | 0.16          |
| (1,1135) | 1:33:A:LYS:HD2  | 1:38:A:VAL:HG12 | 17       | 0.16          |
| (1,1135) | 1:33:A:LYS:HD2  | 1:38:A:VAL:HG13 | 17       | 0.16          |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA2  | 1        | 0.16          |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA3  | 1        | 0.16          |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA2  | 1        | 0.16          |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA3  | 1        | 0.16          |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA2  | 1        | 0.16          |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA3  | 1        | 0.16          |
| (1,1127) | 1:33:A:LYS:HD3  | 1:38:A:VAL:HB   | 12       | 0.16          |
| (1,1127) | 1:33:A:LYS:HD3  | 1:38:A:VAL:HB   | 19       | 0.16          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 11       | 0.16          |
| (1,970)  | 1:25:A:VAL:HG11 | 1:40:A:PRO:HA   | 20       | 0.16          |
| (1,970)  | 1:25:A:VAL:HG12 | 1:40:A:PRO:HA   | 20       | 0.16          |
| (1,970)  | 1:25:A:VAL:HG13 | 1:40:A:PRO:HA   | 20       | 0.16          |
| (1,744)  | 1:2:A:ALA:HA    | 1:3:A:LEU:HG    | 15       | 0.16          |
| (1,655)  | 1:74:A:MET:HA   | 1:76:A:GLY:H    | 11       | 0.16          |
| (1,645)  | 1:44:A:LYS:H    | 1:75:A:MET:H    | 7        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 2        | 0.16          |
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 5        | 0.16          |
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 12       | 0.16          |
| (1,98)   | 1:29:A:LYS:HE2  | 1:30:A:GLN:H    | 18       | 0.16          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 11       | 0.15          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 13       | 0.15          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 19       | 0.15          |
| (1,1717) | 1:43:A:GLN:HG2  | 1:77:A:THR:HB   | 14       | 0.15          |
| (1,1717) | 1:43:A:GLN:HG3  | 1:77:A:THR:HB   | 14       | 0.15          |
| (1,1699) | 1:38:A:VAL:HG11 | 1:76:A:GLY:HA2  | 20       | 0.15          |
| (1,1699) | 1:38:A:VAL:HG11 | 1:76:A:GLY:HA3  | 20       | 0.15          |
| (1,1699) | 1:38:A:VAL:HG12 | 1:76:A:GLY:HA2  | 20       | 0.15          |
| (1,1699) | 1:38:A:VAL:HG12 | 1:76:A:GLY:HA3  | 20       | 0.15          |
| (1,1699) | 1:38:A:VAL:HG13 | 1:76:A:GLY:HA2  | 20       | 0.15          |
| (1,1699) | 1:38:A:VAL:HG13 | 1:76:A:GLY:HA3  | 20       | 0.15          |
| (1,1699) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA2  | 20       | 0.15          |
| (1,1699) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA3  | 20       | 0.15          |
| (1,1699) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA2  | 20       | 0.15          |
| (1,1699) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA3  | 20       | 0.15          |
| (1,1699) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA2  | 20       | 0.15          |
| (1,1699) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA3  | 20       | 0.15          |
| (1,1694) | 1:38:A:VAL:HG11 | 1:43:A:GLN:H    | 1        | 0.15          |
| (1,1694) | 1:38:A:VAL:HG12 | 1:43:A:GLN:H    | 1        | 0.15          |
| (1,1694) | 1:38:A:VAL:HG13 | 1:43:A:GLN:H    | 1        | 0.15          |
| (1,1694) | 1:38:A:VAL:HG21 | 1:43:A:GLN:H    | 1        | 0.15          |
| (1,1694) | 1:38:A:VAL:HG22 | 1:43:A:GLN:H    | 1        | 0.15          |
| (1,1694) | 1:38:A:VAL:HG23 | 1:43:A:GLN:H    | 1        | 0.15          |
| (1,1694) | 1:38:A:VAL:HG11 | 1:43:A:GLN:H    | 17       | 0.15          |
| (1,1694) | 1:38:A:VAL:HG12 | 1:43:A:GLN:H    | 17       | 0.15          |
| (1,1694) | 1:38:A:VAL:HG13 | 1:43:A:GLN:H    | 17       | 0.15          |
| (1,1694) | 1:38:A:VAL:HG21 | 1:43:A:GLN:H    | 17       | 0.15          |
| (1,1694) | 1:38:A:VAL:HG22 | 1:43:A:GLN:H    | 17       | 0.15          |
| (1,1694) | 1:38:A:VAL:HG23 | 1:43:A:GLN:H    | 17       | 0.15          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG21 | 3        | 0.15          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG22 | 3        | 0.15          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG23 | 3        | 0.15          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG21 | 3        | 0.15          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG22 | 3        | 0.15          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG23 | 3        | 0.15          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG21 | 3        | 0.15          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG22 | 3        | 0.15          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG23 | 3        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1264) | 1:59:A:VAL:HA   | 1:64:A:LEU:HG   | 3        | 0.15          |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA2  | 3        | 0.15          |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA3  | 3        | 0.15          |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA2  | 3        | 0.15          |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA3  | 3        | 0.15          |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA2  | 3        | 0.15          |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA3  | 3        | 0.15          |
| (1,1127) | 1:33:A:LYS:HD3  | 1:38:A:VAL:HB   | 7        | 0.15          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 2        | 0.15          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 5        | 0.15          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 6        | 0.15          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 19       | 0.15          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD11 | 8        | 0.15          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD12 | 8        | 0.15          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD13 | 8        | 0.15          |
| (1,972)  | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 20       | 0.15          |
| (1,972)  | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 20       | 0.15          |
| (1,972)  | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 20       | 0.15          |
| (1,876)  | 1:16:A:VAL:HG21 | 1:31:A:PHE:HD1  | 17       | 0.15          |
| (1,876)  | 1:16:A:VAL:HG22 | 1:31:A:PHE:HD1  | 17       | 0.15          |
| (1,876)  | 1:16:A:VAL:HG23 | 1:31:A:PHE:HD1  | 17       | 0.15          |
| (1,844)  | 1:12:A:GLN:HG2  | 1:14:A:TYR:HE1  | 2        | 0.15          |
| (1,844)  | 1:12:A:GLN:HG3  | 1:14:A:TYR:HE1  | 2        | 0.15          |
| (1,744)  | 1:2:A:ALA:HA    | 1:3:A:LEU:HG    | 4        | 0.15          |
| (1,744)  | 1:2:A:ALA:HA    | 1:3:A:LEU:HG    | 6        | 0.15          |
| (1,744)  | 1:2:A:ALA:HA    | 1:3:A:LEU:HG    | 19       | 0.15          |
| (1,731)  | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 1        | 0.15          |
| (1,731)  | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 1        | 0.15          |
| (1,731)  | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 9        | 0.15          |
| (1,731)  | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 9        | 0.15          |
| (1,731)  | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 19       | 0.15          |
| (1,731)  | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 19       | 0.15          |
| (1,655)  | 1:74:A:MET:HA   | 1:76:A:GLY:H    | 6        | 0.15          |
| (1,655)  | 1:74:A:MET:HA   | 1:76:A:GLY:H    | 9        | 0.15          |
| (1,645)  | 1:44:A:LYS:H    | 1:75:A:MET:H    | 14       | 0.15          |
| (1,645)  | 1:44:A:LYS:H    | 1:75:A:MET:H    | 16       | 0.15          |
| (1,626)  | 1:45:A:LEU:HA   | 1:73:A:MET:H    | 14       | 0.15          |
| (1,252)  | 1:7:A:VAL:H     | 1:32:A:LEU:HB2  | 6        | 0.15          |
| (1,252)  | 1:7:A:VAL:H     | 1:32:A:LEU:HB2  | 14       | 0.15          |
| (1,50)   | 1:19:A:LEU:HG   | 1:24:A:THR:H    | 9        | 0.15          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 2        | 0.14          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 15       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,10)   | 1:44:A:LYS:N    | 1:75:A:MET:O    | 14       | 0.14          |
| (1,1705) | 1:38:A:VAL:HG11 | 1:78:A:ARG:HG2  | 18       | 0.14          |
| (1,1705) | 1:38:A:VAL:HG11 | 1:78:A:ARG:HG3  | 18       | 0.14          |
| (1,1705) | 1:38:A:VAL:HG12 | 1:78:A:ARG:HG2  | 18       | 0.14          |
| (1,1705) | 1:38:A:VAL:HG12 | 1:78:A:ARG:HG3  | 18       | 0.14          |
| (1,1705) | 1:38:A:VAL:HG13 | 1:78:A:ARG:HG2  | 18       | 0.14          |
| (1,1705) | 1:38:A:VAL:HG13 | 1:78:A:ARG:HG3  | 18       | 0.14          |
| (1,1705) | 1:38:A:VAL:HG21 | 1:78:A:ARG:HG2  | 18       | 0.14          |
| (1,1705) | 1:38:A:VAL:HG21 | 1:78:A:ARG:HG3  | 18       | 0.14          |
| (1,1705) | 1:38:A:VAL:HG22 | 1:78:A:ARG:HG2  | 18       | 0.14          |
| (1,1705) | 1:38:A:VAL:HG22 | 1:78:A:ARG:HG3  | 18       | 0.14          |
| (1,1705) | 1:38:A:VAL:HG23 | 1:78:A:ARG:HG2  | 18       | 0.14          |
| (1,1705) | 1:38:A:VAL:HG23 | 1:78:A:ARG:HG3  | 18       | 0.14          |
| (1,1694) | 1:38:A:VAL:HG11 | 1:43:A:GLN:H    | 3        | 0.14          |
| (1,1694) | 1:38:A:VAL:HG12 | 1:43:A:GLN:H    | 3        | 0.14          |
| (1,1694) | 1:38:A:VAL:HG13 | 1:43:A:GLN:H    | 3        | 0.14          |
| (1,1694) | 1:38:A:VAL:HG21 | 1:43:A:GLN:H    | 3        | 0.14          |
| (1,1694) | 1:38:A:VAL:HG22 | 1:43:A:GLN:H    | 3        | 0.14          |
| (1,1694) | 1:38:A:VAL:HG23 | 1:43:A:GLN:H    | 3        | 0.14          |
| (1,1687) | 1:38:A:VAL:HG11 | 1:40:A:PRO:HA   | 17       | 0.14          |
| (1,1687) | 1:38:A:VAL:HG12 | 1:40:A:PRO:HA   | 17       | 0.14          |
| (1,1687) | 1:38:A:VAL:HG13 | 1:40:A:PRO:HA   | 17       | 0.14          |
| (1,1687) | 1:38:A:VAL:HG21 | 1:40:A:PRO:HA   | 17       | 0.14          |
| (1,1687) | 1:38:A:VAL:HG22 | 1:40:A:PRO:HA   | 17       | 0.14          |
| (1,1687) | 1:38:A:VAL:HG23 | 1:40:A:PRO:HA   | 17       | 0.14          |
| (1,1436) | 1:77:A:THR:HB   | 1:78:A:ARG:HD2  | 6        | 0.14          |
| (1,1436) | 1:77:A:THR:HB   | 1:78:A:ARG:HD3  | 6        | 0.14          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 2        | 0.14          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 14       | 0.14          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 15       | 0.14          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 18       | 0.14          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG21 | 2        | 0.14          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG22 | 2        | 0.14          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG23 | 2        | 0.14          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG21 | 2        | 0.14          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG22 | 2        | 0.14          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG23 | 2        | 0.14          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG21 | 2        | 0.14          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG22 | 2        | 0.14          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG23 | 2        | 0.14          |
| (1,1264) | 1:59:A:VAL:HA   | 1:64:A:LEU:HG   | 12       | 0.14          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 5        | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1248) | 1:55:A:ALA:HA  | 1:63:A:ALA:HB2  | 5        | 0.14          |
| (1,1248) | 1:55:A:ALA:HA  | 1:63:A:ALA:HB3  | 5        | 0.14          |
| (1,1248) | 1:55:A:ALA:HA  | 1:63:A:ALA:HB1  | 14       | 0.14          |
| (1,1248) | 1:55:A:ALA:HA  | 1:63:A:ALA:HB2  | 14       | 0.14          |
| (1,1248) | 1:55:A:ALA:HA  | 1:63:A:ALA:HB3  | 14       | 0.14          |
| (1,1248) | 1:55:A:ALA:HA  | 1:63:A:ALA:HB1  | 15       | 0.14          |
| (1,1248) | 1:55:A:ALA:HA  | 1:63:A:ALA:HB2  | 15       | 0.14          |
| (1,1248) | 1:55:A:ALA:HA  | 1:63:A:ALA:HB3  | 15       | 0.14          |
| (1,1127) | 1:33:A:LYS:HD3 | 1:38:A:VAL:HB   | 4        | 0.14          |
| (1,1127) | 1:33:A:LYS:HD3 | 1:38:A:VAL:HB   | 16       | 0.14          |
| (1,1084) | 1:33:A:LYS:HD2 | 1:34:A:THR:HB   | 8        | 0.14          |
| (1,1084) | 1:33:A:LYS:HD2 | 1:34:A:THR:HB   | 10       | 0.14          |
| (1,1084) | 1:33:A:LYS:HD2 | 1:34:A:THR:HB   | 14       | 0.14          |
| (1,1084) | 1:33:A:LYS:HD2 | 1:34:A:THR:HB   | 20       | 0.14          |
| (1,744)  | 1:2:A:ALA:HA   | 1:3:A:LEU:HG    | 20       | 0.14          |
| (1,731)  | 1:4:A:PRO:HD2  | 1:69:A:ASN:H    | 15       | 0.14          |
| (1,731)  | 1:4:A:PRO:HD3  | 1:69:A:ASN:H    | 15       | 0.14          |
| (1,731)  | 1:4:A:PRO:HD2  | 1:69:A:ASN:H    | 18       | 0.14          |
| (1,731)  | 1:4:A:PRO:HD3  | 1:69:A:ASN:H    | 18       | 0.14          |
| (1,731)  | 1:4:A:PRO:HD2  | 1:69:A:ASN:H    | 20       | 0.14          |
| (1,731)  | 1:4:A:PRO:HD3  | 1:69:A:ASN:H    | 20       | 0.14          |
| (1,655)  | 1:74:A:MET:HA  | 1:76:A:GLY:H    | 2        | 0.14          |
| (1,655)  | 1:74:A:MET:HA  | 1:76:A:GLY:H    | 14       | 0.14          |
| (1,645)  | 1:44:A:LYS:H   | 1:75:A:MET:H    | 1        | 0.14          |
| (1,645)  | 1:44:A:LYS:H   | 1:75:A:MET:H    | 4        | 0.14          |
| (1,645)  | 1:44:A:LYS:H   | 1:75:A:MET:H    | 11       | 0.14          |
| (1,645)  | 1:44:A:LYS:H   | 1:75:A:MET:H    | 12       | 0.14          |
| (1,645)  | 1:44:A:LYS:H   | 1:75:A:MET:H    | 13       | 0.14          |
| (1,645)  | 1:44:A:LYS:H   | 1:75:A:MET:H    | 15       | 0.14          |
| (1,626)  | 1:45:A:LEU:HA  | 1:73:A:MET:H    | 16       | 0.14          |
| (1,585)  | 1:5:A:ILE:HD11 | 1:66:A:LEU:H    | 4        | 0.14          |
| (1,585)  | 1:5:A:ILE:HD12 | 1:66:A:LEU:H    | 4        | 0.14          |
| (1,585)  | 1:5:A:ILE:HD13 | 1:66:A:LEU:H    | 4        | 0.14          |
| (1,585)  | 1:5:A:ILE:HD11 | 1:66:A:LEU:H    | 11       | 0.14          |
| (1,585)  | 1:5:A:ILE:HD12 | 1:66:A:LEU:H    | 11       | 0.14          |
| (1,585)  | 1:5:A:ILE:HD13 | 1:66:A:LEU:H    | 11       | 0.14          |
| (1,585)  | 1:5:A:ILE:HD11 | 1:66:A:LEU:H    | 19       | 0.14          |
| (1,585)  | 1:5:A:ILE:HD12 | 1:66:A:LEU:H    | 19       | 0.14          |
| (1,585)  | 1:5:A:ILE:HD13 | 1:66:A:LEU:H    | 19       | 0.14          |
| (1,518)  | 1:26:A:LEU:HB2 | 1:57:A:ASN:H    | 7        | 0.14          |
| (1,462)  | 1:45:A:LEU:H   | 1:45:A:LEU:HD21 | 5        | 0.14          |
| (1,462)  | 1:45:A:LEU:H   | 1:45:A:LEU:HD22 | 5        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,462)  | 1:45:A:LEU:H    | 1:45:A:LEU:HD23 | 5        | 0.14          |
| (1,287)  | 1:13:A:GLU:H    | 1:14:A:TYR:HE1  | 2        | 0.14          |
| (1,252)  | 1:7:A:VAL:H     | 1:32:A:LEU:HB2  | 5        | 0.14          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 3        | 0.13          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 6        | 0.13          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 8        | 0.13          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 14       | 0.13          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 16       | 0.13          |
| (1,1722) | 1:44:A:LYS:HG2  | 1:45:A:LEU:H    | 9        | 0.13          |
| (1,1722) | 1:44:A:LYS:HG3  | 1:45:A:LEU:H    | 9        | 0.13          |
| (1,1705) | 1:38:A:VAL:HG11 | 1:78:A:ARG:HG2  | 9        | 0.13          |
| (1,1705) | 1:38:A:VAL:HG11 | 1:78:A:ARG:HG3  | 9        | 0.13          |
| (1,1705) | 1:38:A:VAL:HG12 | 1:78:A:ARG:HG2  | 9        | 0.13          |
| (1,1705) | 1:38:A:VAL:HG12 | 1:78:A:ARG:HG3  | 9        | 0.13          |
| (1,1705) | 1:38:A:VAL:HG13 | 1:78:A:ARG:HG2  | 9        | 0.13          |
| (1,1705) | 1:38:A:VAL:HG13 | 1:78:A:ARG:HG3  | 9        | 0.13          |
| (1,1705) | 1:38:A:VAL:HG21 | 1:78:A:ARG:HG2  | 9        | 0.13          |
| (1,1705) | 1:38:A:VAL:HG21 | 1:78:A:ARG:HG3  | 9        | 0.13          |
| (1,1705) | 1:38:A:VAL:HG22 | 1:78:A:ARG:HG2  | 9        | 0.13          |
| (1,1705) | 1:38:A:VAL:HG22 | 1:78:A:ARG:HG3  | 9        | 0.13          |
| (1,1705) | 1:38:A:VAL:HG23 | 1:78:A:ARG:HG2  | 9        | 0.13          |
| (1,1705) | 1:38:A:VAL:HG23 | 1:78:A:ARG:HG3  | 9        | 0.13          |
| (1,1699) | 1:38:A:VAL:HG11 | 1:76:A:GLY:HA2  | 18       | 0.13          |
| (1,1699) | 1:38:A:VAL:HG11 | 1:76:A:GLY:HA3  | 18       | 0.13          |
| (1,1699) | 1:38:A:VAL:HG12 | 1:76:A:GLY:HA2  | 18       | 0.13          |
| (1,1699) | 1:38:A:VAL:HG12 | 1:76:A:GLY:HA3  | 18       | 0.13          |
| (1,1699) | 1:38:A:VAL:HG13 | 1:76:A:GLY:HA2  | 18       | 0.13          |
| (1,1699) | 1:38:A:VAL:HG13 | 1:76:A:GLY:HA3  | 18       | 0.13          |
| (1,1699) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA2  | 18       | 0.13          |
| (1,1699) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA3  | 18       | 0.13          |
| (1,1699) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA2  | 18       | 0.13          |
| (1,1699) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA3  | 18       | 0.13          |
| (1,1699) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA2  | 18       | 0.13          |
| (1,1699) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA3  | 18       | 0.13          |
| (1,1689) | 1:38:A:VAL:HG11 | 1:42:A:ARG:H    | 11       | 0.13          |
| (1,1689) | 1:38:A:VAL:HG12 | 1:42:A:ARG:H    | 11       | 0.13          |
| (1,1689) | 1:38:A:VAL:HG13 | 1:42:A:ARG:H    | 11       | 0.13          |
| (1,1689) | 1:38:A:VAL:HG21 | 1:42:A:ARG:H    | 11       | 0.13          |
| (1,1689) | 1:38:A:VAL:HG22 | 1:42:A:ARG:H    | 11       | 0.13          |
| (1,1689) | 1:38:A:VAL:HG23 | 1:42:A:ARG:H    | 11       | 0.13          |
| (1,1687) | 1:38:A:VAL:HG11 | 1:40:A:PRO:HA   | 1        | 0.13          |
| (1,1687) | 1:38:A:VAL:HG12 | 1:40:A:PRO:HA   | 1        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1687) | 1:38:A:VAL:HG13 | 1:40:A:PRO:HA   | 1        | 0.13          |
| (1,1687) | 1:38:A:VAL:HG21 | 1:40:A:PRO:HA   | 1        | 0.13          |
| (1,1687) | 1:38:A:VAL:HG22 | 1:40:A:PRO:HA   | 1        | 0.13          |
| (1,1687) | 1:38:A:VAL:HG23 | 1:40:A:PRO:HA   | 1        | 0.13          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 5        | 0.13          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 5        | 0.13          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 5        | 0.13          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 5        | 0.13          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 5        | 0.13          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 5        | 0.13          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 9        | 0.13          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 9        | 0.13          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 9        | 0.13          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 9        | 0.13          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 9        | 0.13          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 9        | 0.13          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 17       | 0.13          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 17       | 0.13          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 17       | 0.13          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 17       | 0.13          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 17       | 0.13          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 17       | 0.13          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 1        | 0.13          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 4        | 0.13          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 5        | 0.13          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 6        | 0.13          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 10       | 0.13          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 19       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG21 | 1        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG22 | 1        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG23 | 1        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG21 | 1        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG22 | 1        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG23 | 1        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG21 | 1        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG22 | 1        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG23 | 1        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG21 | 8        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG22 | 8        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG23 | 8        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG21 | 8        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG22 | 8        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG23 | 8        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG21 | 8        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG22 | 8        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG23 | 8        | 0.13          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG21 | 16       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG22 | 16       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG23 | 16       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG21 | 16       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG22 | 16       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG23 | 16       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG21 | 16       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG22 | 16       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG23 | 16       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG21 | 18       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG22 | 18       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG23 | 18       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG21 | 18       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG22 | 18       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG23 | 18       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG21 | 18       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG22 | 18       | 0.13          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG23 | 18       | 0.13          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 1        | 0.13          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 1        | 0.13          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 1        | 0.13          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 2        | 0.13          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 2        | 0.13          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 2        | 0.13          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 6        | 0.13          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 6        | 0.13          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 6        | 0.13          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 20       | 0.13          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 20       | 0.13          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 20       | 0.13          |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA2  | 2        | 0.13          |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA3  | 2        | 0.13          |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA2  | 2        | 0.13          |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA3  | 2        | 0.13          |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA2  | 2        | 0.13          |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA3  | 2        | 0.13          |
| (1,1127) | 1:33:A:LYS:HD3  | 1:38:A:VAL:HB   | 9        | 0.13          |
| (1,1127) | 1:33:A:LYS:HD3  | 1:38:A:VAL:HB   | 10       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1127) | 1:33:A:LYS:HD3  | 1:38:A:VAL:HB   | 18       | 0.13          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 3        | 0.13          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 7        | 0.13          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 16       | 0.13          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD11 | 12       | 0.13          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD12 | 12       | 0.13          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD13 | 12       | 0.13          |
| (1,972)  | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 10       | 0.13          |
| (1,972)  | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 10       | 0.13          |
| (1,972)  | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 10       | 0.13          |
| (1,744)  | 1:2:A:ALA:HA    | 1:3:A:LEU:HG    | 9        | 0.13          |
| (1,731)  | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 4        | 0.13          |
| (1,731)  | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 4        | 0.13          |
| (1,731)  | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 13       | 0.13          |
| (1,731)  | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 13       | 0.13          |
| (1,655)  | 1:74:A:MET:HA   | 1:76:A:GLY:H    | 1        | 0.13          |
| (1,655)  | 1:74:A:MET:HA   | 1:76:A:GLY:H    | 7        | 0.13          |
| (1,655)  | 1:74:A:MET:HA   | 1:76:A:GLY:H    | 8        | 0.13          |
| (1,655)  | 1:74:A:MET:HA   | 1:76:A:GLY:H    | 16       | 0.13          |
| (1,645)  | 1:44:A:LYS:H    | 1:75:A:MET:H    | 10       | 0.13          |
| (1,585)  | 1:5:A:ILE:HD11  | 1:66:A:LEU:H    | 1        | 0.13          |
| (1,585)  | 1:5:A:ILE:HD12  | 1:66:A:LEU:H    | 1        | 0.13          |
| (1,585)  | 1:5:A:ILE:HD13  | 1:66:A:LEU:H    | 1        | 0.13          |
| (1,585)  | 1:5:A:ILE:HD11  | 1:66:A:LEU:H    | 2        | 0.13          |
| (1,585)  | 1:5:A:ILE:HD12  | 1:66:A:LEU:H    | 2        | 0.13          |
| (1,585)  | 1:5:A:ILE:HD13  | 1:66:A:LEU:H    | 2        | 0.13          |
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 13       | 0.13          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 9        | 0.13          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 9        | 0.13          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 14       | 0.13          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 14       | 0.13          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 19       | 0.13          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 19       | 0.13          |
| (1,252)  | 1:7:A:VAL:H     | 1:32:A:LEU:HB2  | 16       | 0.13          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 1        | 0.12          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 20       | 0.12          |
| (1,1689) | 1:38:A:VAL:HG11 | 1:42:A:ARG:H    | 17       | 0.12          |
| (1,1689) | 1:38:A:VAL:HG12 | 1:42:A:ARG:H    | 17       | 0.12          |
| (1,1689) | 1:38:A:VAL:HG13 | 1:42:A:ARG:H    | 17       | 0.12          |
| (1,1689) | 1:38:A:VAL:HG21 | 1:42:A:ARG:H    | 17       | 0.12          |
| (1,1689) | 1:38:A:VAL:HG22 | 1:42:A:ARG:H    | 17       | 0.12          |
| (1,1689) | 1:38:A:VAL:HG23 | 1:42:A:ARG:H    | 17       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2  | 14       | 0.12          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3  | 14       | 0.12          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2  | 14       | 0.12          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3  | 14       | 0.12          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2  | 14       | 0.12          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3  | 14       | 0.12          |
| (1,1419) | 1:74:A:MET:HA   | 1:75:A:MET:HG3  | 5        | 0.12          |
| (1,1386) | 1:46:A:LEU:HA   | 1:72:A:ILE:HG21 | 19       | 0.12          |
| (1,1386) | 1:46:A:LEU:HA   | 1:72:A:ILE:HG22 | 19       | 0.12          |
| (1,1386) | 1:46:A:LEU:HA   | 1:72:A:ILE:HG23 | 19       | 0.12          |
| (1,1317) | 1:61:A:LEU:HA   | 1:64:A:LEU:HG   | 18       | 0.12          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 7        | 0.12          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 11       | 0.12          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 17       | 0.12          |
| (1,1287) | 1:24:A:THR:HA   | 1:61:A:LEU:HA   | 9        | 0.12          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG21 | 5        | 0.12          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG22 | 5        | 0.12          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG23 | 5        | 0.12          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG21 | 5        | 0.12          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG22 | 5        | 0.12          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG23 | 5        | 0.12          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG21 | 5        | 0.12          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG22 | 5        | 0.12          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG23 | 5        | 0.12          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG21 | 15       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG22 | 15       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG23 | 15       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG21 | 15       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG22 | 15       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG23 | 15       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG21 | 15       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG22 | 15       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG23 | 15       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG21 | 17       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG22 | 17       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG23 | 17       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG21 | 17       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG22 | 17       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG23 | 17       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG21 | 17       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG22 | 17       | 0.12          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG23 | 17       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1264) | 1:59:A:VAL:HA   | 1:64:A:LEU:HG   | 20       | 0.12          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 4        | 0.12          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 4        | 0.12          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 4        | 0.12          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 10       | 0.12          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 10       | 0.12          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 10       | 0.12          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 12       | 0.12          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 12       | 0.12          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 12       | 0.12          |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA2  | 6        | 0.12          |
| (1,1130) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA3  | 6        | 0.12          |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA2  | 6        | 0.12          |
| (1,1130) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA3  | 6        | 0.12          |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA2  | 6        | 0.12          |
| (1,1130) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA3  | 6        | 0.12          |
| (1,1127) | 1:33:A:LYS:HD3  | 1:38:A:VAL:HB   | 14       | 0.12          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 4        | 0.12          |
| (1,1084) | 1:33:A:LYS:HD2  | 1:34:A:THR:HB   | 18       | 0.12          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD11 | 1        | 0.12          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD12 | 1        | 0.12          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD13 | 1        | 0.12          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD11 | 6        | 0.12          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD12 | 6        | 0.12          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD13 | 6        | 0.12          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD11 | 11       | 0.12          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD12 | 11       | 0.12          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD13 | 11       | 0.12          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD11 | 15       | 0.12          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD12 | 15       | 0.12          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD13 | 15       | 0.12          |
| (1,972)  | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 4        | 0.12          |
| (1,972)  | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 4        | 0.12          |
| (1,972)  | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 4        | 0.12          |
| (1,972)  | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 9        | 0.12          |
| (1,972)  | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 9        | 0.12          |
| (1,972)  | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 9        | 0.12          |
| (1,972)  | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 15       | 0.12          |
| (1,972)  | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 15       | 0.12          |
| (1,972)  | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 15       | 0.12          |
| (1,972)  | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 19       | 0.12          |
| (1,972)  | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 19       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,972) | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 19       | 0.12          |
| (1,844) | 1:12:A:GLN:HG2  | 1:14:A:TYR:HE1  | 11       | 0.12          |
| (1,844) | 1:12:A:GLN:HG3  | 1:14:A:TYR:HE1  | 11       | 0.12          |
| (1,731) | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 3        | 0.12          |
| (1,731) | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 3        | 0.12          |
| (1,731) | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 6        | 0.12          |
| (1,731) | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 6        | 0.12          |
| (1,731) | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 11       | 0.12          |
| (1,731) | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 11       | 0.12          |
| (1,731) | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 14       | 0.12          |
| (1,731) | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 14       | 0.12          |
| (1,731) | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 16       | 0.12          |
| (1,731) | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 16       | 0.12          |
| (1,655) | 1:74:A:MET:HA   | 1:76:A:GLY:H    | 4        | 0.12          |
| (1,655) | 1:74:A:MET:HA   | 1:76:A:GLY:H    | 12       | 0.12          |
| (1,655) | 1:74:A:MET:HA   | 1:76:A:GLY:H    | 19       | 0.12          |
| (1,597) | 1:4:A:PRO:HG2   | 1:69:A:ASN:H    | 16       | 0.12          |
| (1,585) | 1:5:A:ILE:HD11  | 1:66:A:LEU:H    | 6        | 0.12          |
| (1,585) | 1:5:A:ILE:HD12  | 1:66:A:LEU:H    | 6        | 0.12          |
| (1,585) | 1:5:A:ILE:HD13  | 1:66:A:LEU:H    | 6        | 0.12          |
| (1,585) | 1:5:A:ILE:HD11  | 1:66:A:LEU:H    | 13       | 0.12          |
| (1,585) | 1:5:A:ILE:HD12  | 1:66:A:LEU:H    | 13       | 0.12          |
| (1,585) | 1:5:A:ILE:HD13  | 1:66:A:LEU:H    | 13       | 0.12          |
| (1,585) | 1:5:A:ILE:HD11  | 1:66:A:LEU:H    | 18       | 0.12          |
| (1,585) | 1:5:A:ILE:HD12  | 1:66:A:LEU:H    | 18       | 0.12          |
| (1,585) | 1:5:A:ILE:HD13  | 1:66:A:LEU:H    | 18       | 0.12          |
| (1,518) | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 3        | 0.12          |
| (1,518) | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 6        | 0.12          |
| (1,518) | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 16       | 0.12          |
| (1,471) | 1:46:A:LEU:H    | 1:74:A:MET:HG3  | 18       | 0.12          |
| (1,464) | 1:46:A:LEU:H    | 1:74:A:MET:HA   | 9        | 0.12          |
| (1,462) | 1:45:A:LEU:H    | 1:45:A:LEU:HD21 | 14       | 0.12          |
| (1,462) | 1:45:A:LEU:H    | 1:45:A:LEU:HD22 | 14       | 0.12          |
| (1,462) | 1:45:A:LEU:H    | 1:45:A:LEU:HD23 | 14       | 0.12          |
| (1,462) | 1:45:A:LEU:H    | 1:45:A:LEU:HD21 | 16       | 0.12          |
| (1,462) | 1:45:A:LEU:H    | 1:45:A:LEU:HD22 | 16       | 0.12          |
| (1,462) | 1:45:A:LEU:H    | 1:45:A:LEU:HD23 | 16       | 0.12          |
| (1,330) | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 1        | 0.12          |
| (1,330) | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 1        | 0.12          |
| (1,252) | 1:7:A:VAL:H     | 1:32:A:LEU:HB2  | 4        | 0.12          |
| (1,252) | 1:7:A:VAL:H     | 1:32:A:LEU:HB2  | 12       | 0.12          |
| (2,26)  | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 18       | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (2,23)   | 1:30:A:GLN:O    | 1:34:A:THR:H   | 3        | 0.11          |
| (1,1699) | 1:38:A:VAL:HG11 | 1:76:A:GLY:HA2 | 9        | 0.11          |
| (1,1699) | 1:38:A:VAL:HG11 | 1:76:A:GLY:HA3 | 9        | 0.11          |
| (1,1699) | 1:38:A:VAL:HG12 | 1:76:A:GLY:HA2 | 9        | 0.11          |
| (1,1699) | 1:38:A:VAL:HG12 | 1:76:A:GLY:HA3 | 9        | 0.11          |
| (1,1699) | 1:38:A:VAL:HG13 | 1:76:A:GLY:HA2 | 9        | 0.11          |
| (1,1699) | 1:38:A:VAL:HG13 | 1:76:A:GLY:HA3 | 9        | 0.11          |
| (1,1699) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA2 | 9        | 0.11          |
| (1,1699) | 1:38:A:VAL:HG21 | 1:76:A:GLY:HA3 | 9        | 0.11          |
| (1,1699) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA2 | 9        | 0.11          |
| (1,1699) | 1:38:A:VAL:HG22 | 1:76:A:GLY:HA3 | 9        | 0.11          |
| (1,1699) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA2 | 9        | 0.11          |
| (1,1699) | 1:38:A:VAL:HG23 | 1:76:A:GLY:HA3 | 9        | 0.11          |
| (1,1694) | 1:38:A:VAL:HG11 | 1:43:A:GLN:H   | 2        | 0.11          |
| (1,1694) | 1:38:A:VAL:HG12 | 1:43:A:GLN:H   | 2        | 0.11          |
| (1,1694) | 1:38:A:VAL:HG13 | 1:43:A:GLN:H   | 2        | 0.11          |
| (1,1694) | 1:38:A:VAL:HG21 | 1:43:A:GLN:H   | 2        | 0.11          |
| (1,1694) | 1:38:A:VAL:HG22 | 1:43:A:GLN:H   | 2        | 0.11          |
| (1,1694) | 1:38:A:VAL:HG23 | 1:43:A:GLN:H   | 2        | 0.11          |
| (1,1687) | 1:38:A:VAL:HG11 | 1:40:A:PRO:HA  | 8        | 0.11          |
| (1,1687) | 1:38:A:VAL:HG12 | 1:40:A:PRO:HA  | 8        | 0.11          |
| (1,1687) | 1:38:A:VAL:HG13 | 1:40:A:PRO:HA  | 8        | 0.11          |
| (1,1687) | 1:38:A:VAL:HG21 | 1:40:A:PRO:HA  | 8        | 0.11          |
| (1,1687) | 1:38:A:VAL:HG22 | 1:40:A:PRO:HA  | 8        | 0.11          |
| (1,1687) | 1:38:A:VAL:HG23 | 1:40:A:PRO:HA  | 8        | 0.11          |
| (1,1549) | 1:8:A:LYS:HE2   | 1:9:A:TRP:H    | 8        | 0.11          |
| (1,1549) | 1:8:A:LYS:HE3   | 1:9:A:TRP:H    | 8        | 0.11          |
| (1,1482) | 1:68:A:PRO:HA   | 1:70:A:THR:HB  | 4        | 0.11          |
| (1,1482) | 1:68:A:PRO:HA   | 1:70:A:THR:HB  | 6        | 0.11          |
| (1,1482) | 1:68:A:PRO:HA   | 1:70:A:THR:HB  | 7        | 0.11          |
| (1,1482) | 1:68:A:PRO:HA   | 1:70:A:THR:HB  | 9        | 0.11          |
| (1,1482) | 1:68:A:PRO:HA   | 1:70:A:THR:HB  | 10       | 0.11          |
| (1,1482) | 1:68:A:PRO:HA   | 1:70:A:THR:HB  | 20       | 0.11          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD2 | 3        | 0.11          |
| (1,1466) | 1:25:A:VAL:HG11 | 1:40:A:PRO:HD3 | 3        | 0.11          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD2 | 3        | 0.11          |
| (1,1466) | 1:25:A:VAL:HG12 | 1:40:A:PRO:HD3 | 3        | 0.11          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD2 | 3        | 0.11          |
| (1,1466) | 1:25:A:VAL:HG13 | 1:40:A:PRO:HD3 | 3        | 0.11          |
| (1,1317) | 1:61:A:LEU:HA   | 1:64:A:LEU:HG  | 2        | 0.11          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA  | 9        | 0.11          |
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA  | 13       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1303) | 1:60:A:LYS:HG3  | 1:63:A:ALA:HA   | 16       | 0.11          |
| (1,1287) | 1:24:A:THR:HA   | 1:61:A:LEU:HA   | 2        | 0.11          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG21 | 10       | 0.11          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG22 | 10       | 0.11          |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG23 | 10       | 0.11          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG21 | 10       | 0.11          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG22 | 10       | 0.11          |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG23 | 10       | 0.11          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG21 | 10       | 0.11          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG22 | 10       | 0.11          |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG23 | 10       | 0.11          |
| (1,1264) | 1:59:A:VAL:HA   | 1:64:A:LEU:HG   | 11       | 0.11          |
| (1,1264) | 1:59:A:VAL:HA   | 1:64:A:LEU:HG   | 17       | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 3        | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 3        | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 3        | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 7        | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 7        | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 7        | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 11       | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 11       | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 11       | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 13       | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 13       | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 13       | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 16       | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 16       | 0.11          |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 16       | 0.11          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB2  | 17       | 0.11          |
| (1,1126) | 1:38:A:VAL:HB   | 1:43:A:GLN:HB3  | 17       | 0.11          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD11 | 4        | 0.11          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD12 | 4        | 0.11          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD13 | 4        | 0.11          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD11 | 7        | 0.11          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD12 | 7        | 0.11          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD13 | 7        | 0.11          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD11 | 13       | 0.11          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD12 | 13       | 0.11          |
| (1,1069) | 1:33:A:LYS:HG3  | 1:39:A:LEU:HD13 | 13       | 0.11          |
| (1,972)  | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 1        | 0.11          |
| (1,972)  | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 1        | 0.11          |
| (1,972)  | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 1        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,972) | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 3        | 0.11          |
| (1,972) | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 3        | 0.11          |
| (1,972) | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 3        | 0.11          |
| (1,972) | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 11       | 0.11          |
| (1,972) | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 11       | 0.11          |
| (1,972) | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 11       | 0.11          |
| (1,972) | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 17       | 0.11          |
| (1,972) | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 17       | 0.11          |
| (1,972) | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 17       | 0.11          |
| (1,865) | 1:15:A:SER:HA   | 1:32:A:LEU:HD21 | 9        | 0.11          |
| (1,865) | 1:15:A:SER:HA   | 1:32:A:LEU:HD22 | 9        | 0.11          |
| (1,865) | 1:15:A:SER:HA   | 1:32:A:LEU:HD23 | 9        | 0.11          |
| (1,756) | 1:4:A:PRO:HD2   | 1:5:A:ILE:HA    | 1        | 0.11          |
| (1,756) | 1:4:A:PRO:HD3   | 1:5:A:ILE:HA    | 1        | 0.11          |
| (1,731) | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 5        | 0.11          |
| (1,731) | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 5        | 0.11          |
| (1,731) | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 7        | 0.11          |
| (1,731) | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 7        | 0.11          |
| (1,731) | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 8        | 0.11          |
| (1,731) | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 8        | 0.11          |
| (1,731) | 1:4:A:PRO:HD2   | 1:69:A:ASN:H    | 10       | 0.11          |
| (1,731) | 1:4:A:PRO:HD3   | 1:69:A:ASN:H    | 10       | 0.11          |
| (1,645) | 1:44:A:LYS:H    | 1:75:A:MET:H    | 2        | 0.11          |
| (1,645) | 1:44:A:LYS:H    | 1:75:A:MET:H    | 3        | 0.11          |
| (1,645) | 1:44:A:LYS:H    | 1:75:A:MET:H    | 17       | 0.11          |
| (1,597) | 1:4:A:PRO:HG2   | 1:69:A:ASN:H    | 5        | 0.11          |
| (1,597) | 1:4:A:PRO:HG2   | 1:69:A:ASN:H    | 8        | 0.11          |
| (1,597) | 1:4:A:PRO:HG2   | 1:69:A:ASN:H    | 11       | 0.11          |
| (1,591) | 1:5:A:ILE:HD11  | 1:67:A:LYS:H    | 1        | 0.11          |
| (1,591) | 1:5:A:ILE:HD12  | 1:67:A:LYS:H    | 1        | 0.11          |
| (1,591) | 1:5:A:ILE:HD13  | 1:67:A:LYS:H    | 1        | 0.11          |
| (1,591) | 1:5:A:ILE:HD11  | 1:67:A:LYS:H    | 5        | 0.11          |
| (1,591) | 1:5:A:ILE:HD12  | 1:67:A:LYS:H    | 5        | 0.11          |
| (1,591) | 1:5:A:ILE:HD13  | 1:67:A:LYS:H    | 5        | 0.11          |
| (1,585) | 1:5:A:ILE:HD11  | 1:66:A:LEU:H    | 8        | 0.11          |
| (1,585) | 1:5:A:ILE:HD12  | 1:66:A:LEU:H    | 8        | 0.11          |
| (1,585) | 1:5:A:ILE:HD13  | 1:66:A:LEU:H    | 8        | 0.11          |
| (1,585) | 1:5:A:ILE:HD11  | 1:66:A:LEU:H    | 9        | 0.11          |
| (1,585) | 1:5:A:ILE:HD12  | 1:66:A:LEU:H    | 9        | 0.11          |
| (1,585) | 1:5:A:ILE:HD13  | 1:66:A:LEU:H    | 9        | 0.11          |
| (1,585) | 1:5:A:ILE:HD11  | 1:66:A:LEU:H    | 10       | 0.11          |
| (1,585) | 1:5:A:ILE:HD12  | 1:66:A:LEU:H    | 10       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,585)  | 1:5:A:ILE:HD13  | 1:66:A:LEU:H    | 10       | 0.11          |
| (1,585)  | 1:5:A:ILE:HD11  | 1:66:A:LEU:H    | 15       | 0.11          |
| (1,585)  | 1:5:A:ILE:HD12  | 1:66:A:LEU:H    | 15       | 0.11          |
| (1,585)  | 1:5:A:ILE:HD13  | 1:66:A:LEU:H    | 15       | 0.11          |
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 4        | 0.11          |
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 11       | 0.11          |
| (1,518)  | 1:26:A:LEU:HB2  | 1:57:A:ASN:H    | 19       | 0.11          |
| (1,454)  | 1:29:A:LYS:HE2  | 1:45:A:LEU:H    | 20       | 0.11          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 4        | 0.11          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 4        | 0.11          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 6        | 0.11          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 6        | 0.11          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB2  | 17       | 0.11          |
| (1,330)  | 1:19:A:LEU:H    | 1:23:A:ASP:HB3  | 17       | 0.11          |
| (1,269)  | 1:8:A:LYS:H     | 1:32:A:LEU:HD21 | 5        | 0.11          |
| (1,269)  | 1:8:A:LYS:H     | 1:32:A:LEU:HD22 | 5        | 0.11          |
| (1,269)  | 1:8:A:LYS:H     | 1:32:A:LEU:HD23 | 5        | 0.11          |
| (1,269)  | 1:8:A:LYS:H     | 1:32:A:LEU:HD21 | 14       | 0.11          |
| (1,269)  | 1:8:A:LYS:H     | 1:32:A:LEU:HD22 | 14       | 0.11          |
| (1,269)  | 1:8:A:LYS:H     | 1:32:A:LEU:HD23 | 14       | 0.11          |
| (1,258)  | 1:7:A:VAL:H     | 1:32:A:LEU:HD21 | 6        | 0.11          |
| (1,258)  | 1:7:A:VAL:H     | 1:32:A:LEU:HD22 | 6        | 0.11          |
| (1,258)  | 1:7:A:VAL:H     | 1:32:A:LEU:HD23 | 6        | 0.11          |
| (1,252)  | 1:7:A:VAL:H     | 1:32:A:LEU:HB2  | 3        | 0.11          |
| (1,252)  | 1:7:A:VAL:H     | 1:32:A:LEU:HB2  | 19       | 0.11          |
| (1,220)  | 1:3:A:LEU:H     | 1:21:A:GLU:H    | 9        | 0.11          |
| (1,210)  | 1:26:A:LEU:H    | 1:26:A:LEU:HB2  | 6        | 0.11          |
| (1,210)  | 1:26:A:LEU:H    | 1:26:A:LEU:HB2  | 19       | 0.11          |
| (1,180)  | 1:33:A:LYS:HA   | 1:38:A:VAL:H    | 17       | 0.11          |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 5        | 0.1           |
| (2,26)   | 1:31:A:PHE:O    | 1:35:A:LEU:N    | 17       | 0.1           |
| (2,18)   | 1:27:A:ASP:O    | 1:31:A:PHE:N    | 4        | 0.1           |
| (2,18)   | 1:27:A:ASP:O    | 1:31:A:PHE:N    | 10       | 0.1           |
| (1,1694) | 1:38:A:VAL:HG11 | 1:43:A:GLN:H    | 8        | 0.1           |
| (1,1694) | 1:38:A:VAL:HG12 | 1:43:A:GLN:H    | 8        | 0.1           |
| (1,1694) | 1:38:A:VAL:HG13 | 1:43:A:GLN:H    | 8        | 0.1           |
| (1,1694) | 1:38:A:VAL:HG21 | 1:43:A:GLN:H    | 8        | 0.1           |
| (1,1694) | 1:38:A:VAL:HG22 | 1:43:A:GLN:H    | 8        | 0.1           |
| (1,1694) | 1:38:A:VAL:HG23 | 1:43:A:GLN:H    | 8        | 0.1           |
| (1,1482) | 1:68:A:PRO:HA   | 1:70:A:THR:HB   | 5        | 0.1           |
| (1,1482) | 1:68:A:PRO:HA   | 1:70:A:THR:HB   | 12       | 0.1           |
| (1,1317) | 1:61:A:LEU:HA   | 1:64:A:LEU:HG   | 9        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1317) | 1:61:A:LEU:HA   | 1:64:A:LEU:HG   | 10       | 0.1           |
| (1,1317) | 1:61:A:LEU:HA   | 1:64:A:LEU:HG   | 11       | 0.1           |
| (1,1287) | 1:24:A:THR:HA   | 1:61:A:LEU:HA   | 18       | 0.1           |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG21 | 4        | 0.1           |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG22 | 4        | 0.1           |
| (1,1268) | 1:55:A:ALA:HB1  | 1:59:A:VAL:HG23 | 4        | 0.1           |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG21 | 4        | 0.1           |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG22 | 4        | 0.1           |
| (1,1268) | 1:55:A:ALA:HB2  | 1:59:A:VAL:HG23 | 4        | 0.1           |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG21 | 4        | 0.1           |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG22 | 4        | 0.1           |
| (1,1268) | 1:55:A:ALA:HB3  | 1:59:A:VAL:HG23 | 4        | 0.1           |
| (1,1264) | 1:59:A:VAL:HA   | 1:64:A:LEU:HG   | 10       | 0.1           |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 17       | 0.1           |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 17       | 0.1           |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 17       | 0.1           |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB1  | 19       | 0.1           |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB2  | 19       | 0.1           |
| (1,1248) | 1:55:A:ALA:HA   | 1:63:A:ALA:HB3  | 19       | 0.1           |
| (1,1200) | 1:46:A:LEU:HB2  | 1:46:A:LEU:HG   | 5        | 0.1           |
| (1,983)  | 1:26:A:LEU:HA   | 1:26:A:LEU:HG   | 6        | 0.1           |
| (1,983)  | 1:26:A:LEU:HA   | 1:26:A:LEU:HG   | 10       | 0.1           |
| (1,983)  | 1:26:A:LEU:HA   | 1:26:A:LEU:HG   | 11       | 0.1           |
| (1,983)  | 1:26:A:LEU:HA   | 1:26:A:LEU:HG   | 19       | 0.1           |
| (1,972)  | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 5        | 0.1           |
| (1,972)  | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 5        | 0.1           |
| (1,972)  | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 5        | 0.1           |
| (1,972)  | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 7        | 0.1           |
| (1,972)  | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 7        | 0.1           |
| (1,972)  | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 7        | 0.1           |
| (1,972)  | 1:25:A:VAL:HG21 | 1:29:A:LYS:HE3  | 12       | 0.1           |
| (1,972)  | 1:25:A:VAL:HG22 | 1:29:A:LYS:HE3  | 12       | 0.1           |
| (1,972)  | 1:25:A:VAL:HG23 | 1:29:A:LYS:HE3  | 12       | 0.1           |
| (1,854)  | 1:14:A:TYR:HB2  | 1:14:A:TYR:HE1  | 9        | 0.1           |
| (1,756)  | 1:4:A:PRO:HD2   | 1:5:A:ILE:HA    | 2        | 0.1           |
| (1,756)  | 1:4:A:PRO:HD3   | 1:5:A:ILE:HA    | 2        | 0.1           |
| (1,756)  | 1:4:A:PRO:HD2   | 1:5:A:ILE:HA    | 9        | 0.1           |
| (1,756)  | 1:4:A:PRO:HD3   | 1:5:A:ILE:HA    | 9        | 0.1           |
| (1,756)  | 1:4:A:PRO:HD2   | 1:5:A:ILE:HA    | 16       | 0.1           |
| (1,756)  | 1:4:A:PRO:HD3   | 1:5:A:ILE:HA    | 16       | 0.1           |
| (1,756)  | 1:4:A:PRO:HD2   | 1:5:A:ILE:HA    | 17       | 0.1           |
| (1,756)  | 1:4:A:PRO:HD3   | 1:5:A:ILE:HA    | 17       | 0.1           |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,756) | 1:4:A:PRO:HD2   | 1:5:A:ILE:HA   | 18       | 0.1           |
| (1,756) | 1:4:A:PRO:HD3   | 1:5:A:ILE:HA   | 18       | 0.1           |
| (1,756) | 1:4:A:PRO:HD2   | 1:5:A:ILE:HA   | 19       | 0.1           |
| (1,756) | 1:4:A:PRO:HD3   | 1:5:A:ILE:HA   | 19       | 0.1           |
| (1,756) | 1:4:A:PRO:HD2   | 1:5:A:ILE:HA   | 20       | 0.1           |
| (1,756) | 1:4:A:PRO:HD3   | 1:5:A:ILE:HA   | 20       | 0.1           |
| (1,738) | 1:25:A:VAL:HG11 | 1:55:A:ALA:HB1 | 19       | 0.1           |
| (1,738) | 1:25:A:VAL:HG11 | 1:55:A:ALA:HB2 | 19       | 0.1           |
| (1,738) | 1:25:A:VAL:HG11 | 1:55:A:ALA:HB3 | 19       | 0.1           |
| (1,738) | 1:25:A:VAL:HG12 | 1:55:A:ALA:HB1 | 19       | 0.1           |
| (1,738) | 1:25:A:VAL:HG12 | 1:55:A:ALA:HB2 | 19       | 0.1           |
| (1,738) | 1:25:A:VAL:HG12 | 1:55:A:ALA:HB3 | 19       | 0.1           |
| (1,738) | 1:25:A:VAL:HG13 | 1:55:A:ALA:HB1 | 19       | 0.1           |
| (1,738) | 1:25:A:VAL:HG13 | 1:55:A:ALA:HB2 | 19       | 0.1           |
| (1,738) | 1:25:A:VAL:HG13 | 1:55:A:ALA:HB3 | 19       | 0.1           |
| (1,731) | 1:4:A:PRO:HD2   | 1:69:A:ASN:H   | 2        | 0.1           |
| (1,731) | 1:4:A:PRO:HD3   | 1:69:A:ASN:H   | 2        | 0.1           |
| (1,731) | 1:4:A:PRO:HD2   | 1:69:A:ASN:H   | 12       | 0.1           |
| (1,731) | 1:4:A:PRO:HD3   | 1:69:A:ASN:H   | 12       | 0.1           |
| (1,731) | 1:4:A:PRO:HD2   | 1:69:A:ASN:H   | 17       | 0.1           |
| (1,731) | 1:4:A:PRO:HD3   | 1:69:A:ASN:H   | 17       | 0.1           |
| (1,655) | 1:74:A:MET:HA   | 1:76:A:GLY:H   | 15       | 0.1           |
| (1,655) | 1:74:A:MET:HA   | 1:76:A:GLY:H   | 20       | 0.1           |
| (1,651) | 1:45:A:LEU:HA   | 1:75:A:MET:H   | 20       | 0.1           |
| (1,645) | 1:44:A:LYS:H    | 1:75:A:MET:H   | 8        | 0.1           |
| (1,626) | 1:45:A:LEU:HA   | 1:73:A:MET:H   | 17       | 0.1           |
| (1,597) | 1:4:A:PRO:HG2   | 1:69:A:ASN:H   | 2        | 0.1           |
| (1,591) | 1:5:A:ILE:HD11  | 1:67:A:LYS:H   | 3        | 0.1           |
| (1,591) | 1:5:A:ILE:HD12  | 1:67:A:LYS:H   | 3        | 0.1           |
| (1,591) | 1:5:A:ILE:HD13  | 1:67:A:LYS:H   | 3        | 0.1           |
| (1,591) | 1:5:A:ILE:HD11  | 1:67:A:LYS:H   | 16       | 0.1           |
| (1,591) | 1:5:A:ILE:HD12  | 1:67:A:LYS:H   | 16       | 0.1           |
| (1,591) | 1:5:A:ILE:HD13  | 1:67:A:LYS:H   | 16       | 0.1           |
| (1,591) | 1:5:A:ILE:HD11  | 1:67:A:LYS:H   | 17       | 0.1           |
| (1,591) | 1:5:A:ILE:HD12  | 1:67:A:LYS:H   | 17       | 0.1           |
| (1,591) | 1:5:A:ILE:HD13  | 1:67:A:LYS:H   | 17       | 0.1           |
| (1,585) | 1:5:A:ILE:HD11  | 1:66:A:LEU:H   | 12       | 0.1           |
| (1,585) | 1:5:A:ILE:HD12  | 1:66:A:LEU:H   | 12       | 0.1           |
| (1,585) | 1:5:A:ILE:HD13  | 1:66:A:LEU:H   | 12       | 0.1           |
| (1,330) | 1:19:A:LEU:H    | 1:23:A:ASP:HB2 | 10       | 0.1           |
| (1,330) | 1:19:A:LEU:H    | 1:23:A:ASP:HB3 | 10       | 0.1           |
| (1,330) | 1:19:A:LEU:H    | 1:23:A:ASP:HB2 | 11       | 0.1           |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,330) | 1:19:A:LEU:H    | 1:23:A:ASP:HB3 | 11       | 0.1           |
| (1,330) | 1:19:A:LEU:H    | 1:23:A:ASP:HB2 | 12       | 0.1           |
| (1,330) | 1:19:A:LEU:H    | 1:23:A:ASP:HB3 | 12       | 0.1           |
| (1,230) | 1:39:A:LEU:HD21 | 1:79:A:GLU:H   | 13       | 0.1           |
| (1,230) | 1:39:A:LEU:HD22 | 1:79:A:GLU:H   | 13       | 0.1           |
| (1,230) | 1:39:A:LEU:HD23 | 1:79:A:GLU:H   | 13       | 0.1           |
| (1,210) | 1:26:A:LEU:H    | 1:26:A:LEU:HB2 | 4        | 0.1           |
| (1,210) | 1:26:A:LEU:H    | 1:26:A:LEU:HB2 | 10       | 0.1           |
| (1,210) | 1:26:A:LEU:H    | 1:26:A:LEU:HB2 | 11       | 0.1           |
| (1,190) | 1:33:A:LYS:HB2  | 1:38:A:VAL:H   | 1        | 0.1           |
| (1,50)  | 1:19:A:LEU:HG   | 1:24:A:THR:H   | 11       | 0.1           |
| (1,20)  | 1:60:A:LYS:HG3  | 1:63:A:ALA:H   | 17       | 0.1           |

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

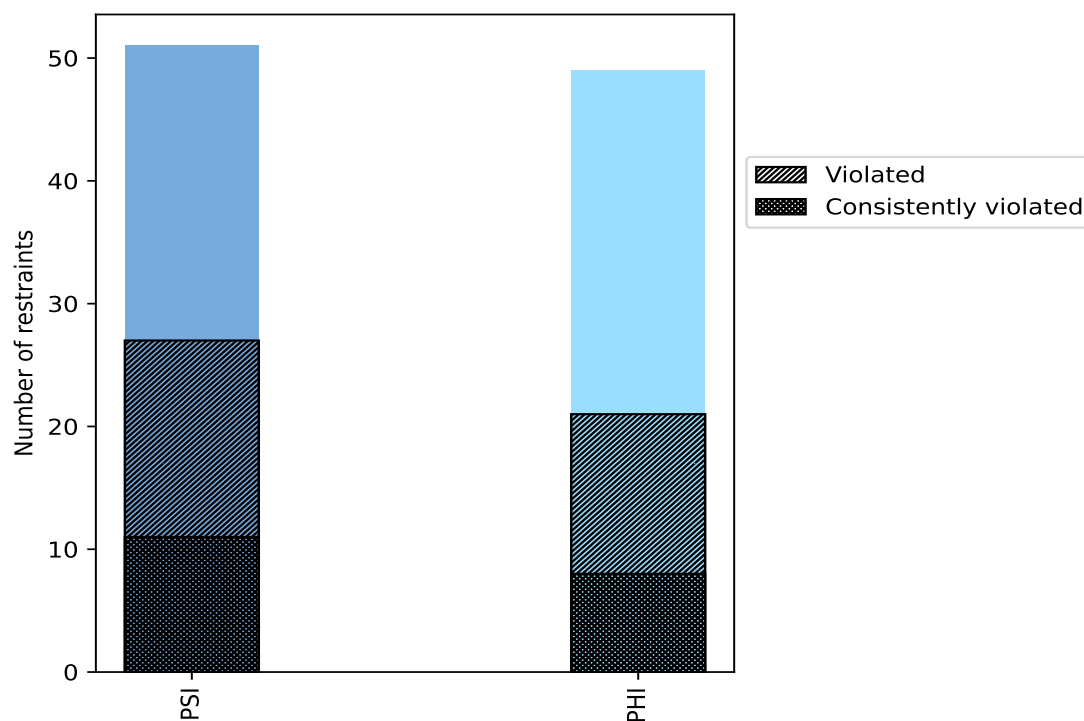
### 10.1 Summary of dihedral-angle violations [i](#)

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        | 51    | 51.0           | 27                    | 52.9           | 27.0           | 11                                 | 21.6           | 11.0           |
| PHI        | 49    | 49.0           | 21                    | 42.9           | 21.0           | 8                                  | 16.3           | 8.0            |
| Total      | 100   | 100.0          | 48                    | 48.0           | 48.0           | 19                                 | 19.0           | 19.0           |

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

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



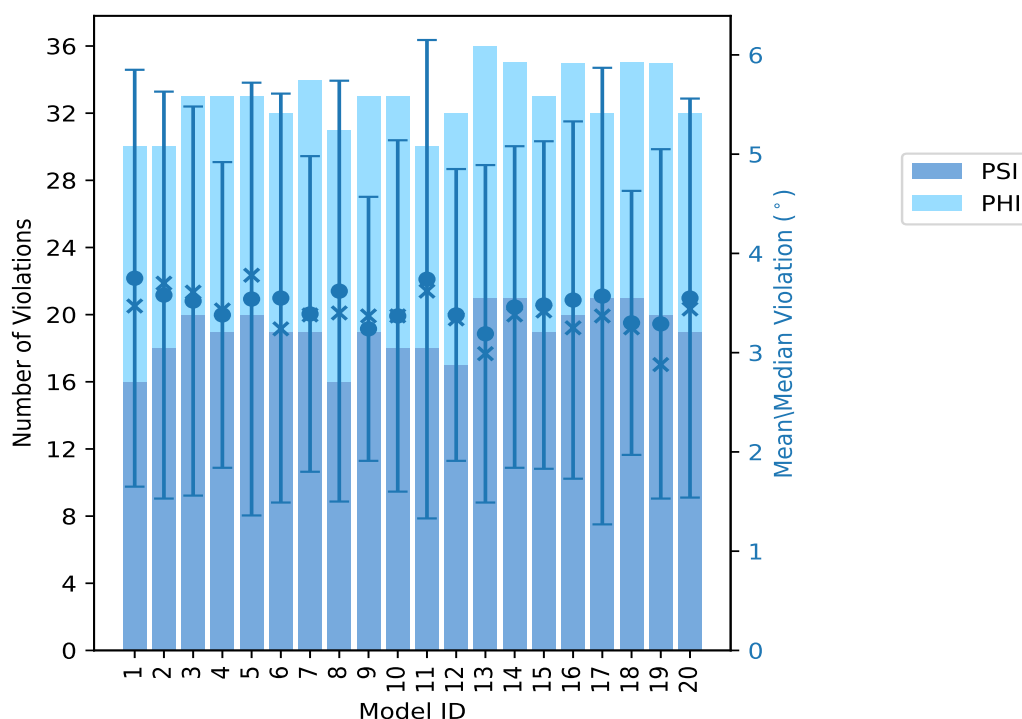
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 16                   | 14  | 30    | 3.75     | 9.34    | 2.1    | 3.47       |
| 2        | 18                   | 12  | 30    | 3.58     | 9.51    | 2.05   | 3.7        |
| 3        | 20                   | 13  | 33    | 3.52     | 8.44    | 1.96   | 3.61       |
| 4        | 19                   | 14  | 33    | 3.38     | 6.77    | 1.54   | 3.43       |
| 5        | 20                   | 13  | 33    | 3.54     | 10.0    | 2.18   | 3.78       |
| 6        | 19                   | 13  | 32    | 3.55     | 8.8     | 2.06   | 3.24       |
| 7        | 19                   | 15  | 34    | 3.39     | 7.1     | 1.59   | 3.38       |
| 8        | 16                   | 15  | 31    | 3.62     | 9.99    | 2.12   | 3.4        |
| 9        | 19                   | 14  | 33    | 3.24     | 5.8     | 1.33   | 3.37       |
| 10       | 18                   | 15  | 33    | 3.37     | 7.19    | 1.77   | 3.37       |
| 11       | 18                   | 12  | 30    | 3.74     | 10.86   | 2.41   | 3.62       |
| 12       | 17                   | 15  | 32    | 3.38     | 7.01    | 1.47   | 3.34       |
| 13       | 21                   | 15  | 36    | 3.19     | 6.89    | 1.7    | 2.99       |
| 14       | 21                   | 14  | 35    | 3.46     | 6.74    | 1.62   | 3.38       |
| 15       | 19                   | 14  | 33    | 3.48     | 7.11    | 1.65   | 3.42       |
| 16       | 20                   | 15  | 35    | 3.53     | 7.53    | 1.8    | 3.25       |
| 17       | 21                   | 11  | 32    | 3.57     | 10.44   | 2.3    | 3.37       |
| 18       | 21                   | 14  | 35    | 3.3      | 5.92    | 1.33   | 3.25       |
| 19       | 20                   | 15  | 35    | 3.29     | 7.1     | 1.76   | 2.88       |
| 20       | 19                   | 13  | 32    | 3.55     | 9.63    | 2.01   | 3.44       |

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

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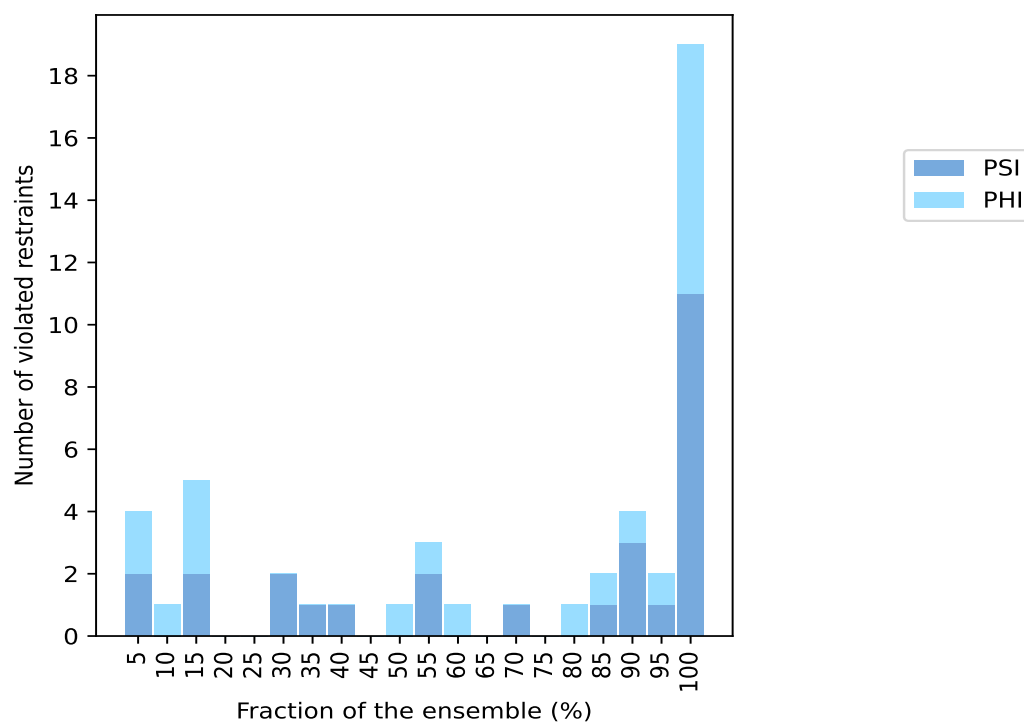


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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 1   | 1     | 12                       | 60.0  |
| 0                             | 0   | 0     | 13                       | 65.0  |
| 1                             | 0   | 1     | 14                       | 70.0  |
| 0                             | 0   | 0     | 15                       | 75.0  |
| 0                             | 1   | 1     | 16                       | 80.0  |
| 1                             | 1   | 2     | 17                       | 85.0  |
| 3                             | 1   | 4     | 18                       | 90.0  |
| 1                             | 1   | 2     | 19                       | 95.0  |
| 11                            | 8   | 19    | 20                       | 100.0 |

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

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

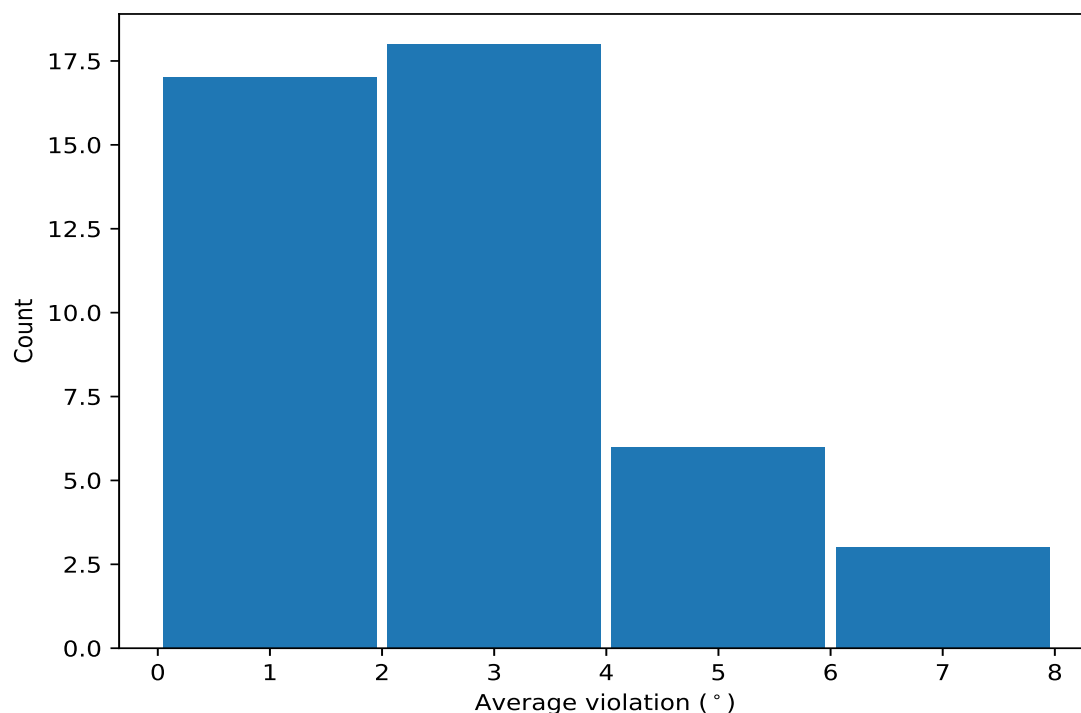


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 20                  | 7.18 | 2.38            | 6.98   |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 20                  | 7.13 | 1.57            | 7.1    |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 20                  | 6.64 | 1.5             | 6.6    |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 20                  | 5.69 | 1.06            | 5.74   |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 20                  | 5.5  | 0.92            | 5.48   |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 20                  | 5.11 | 0.31            | 5.12   |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 20                  | 4.62 | 0.48            | 4.58   |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 20                  | 4.29 | 0.61            | 4.16   |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 20                  | 3.95 | 0.74            | 3.91   |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 20                  | 3.9  | 0.61            | 3.9    |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 20                  | 3.79 | 0.23            | 3.78   |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 20                  | 3.74 | 0.5             | 3.78   |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 20                  | 3.74 | 0.21            | 3.69   |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 20                  | 3.67 | 0.6             | 3.5    |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 20                  | 3.44 | 0.52            | 3.4    |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 20                  | 3.25 | 0.39            | 3.34   |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 20                  | 2.85 | 0.42            | 2.8    |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 20                  | 2.05 | 0.66            | 2.14   |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 20                  | 1.63 | 0.21            | 1.67   |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 19                  | 3.78 | 0.46            | 3.86   |

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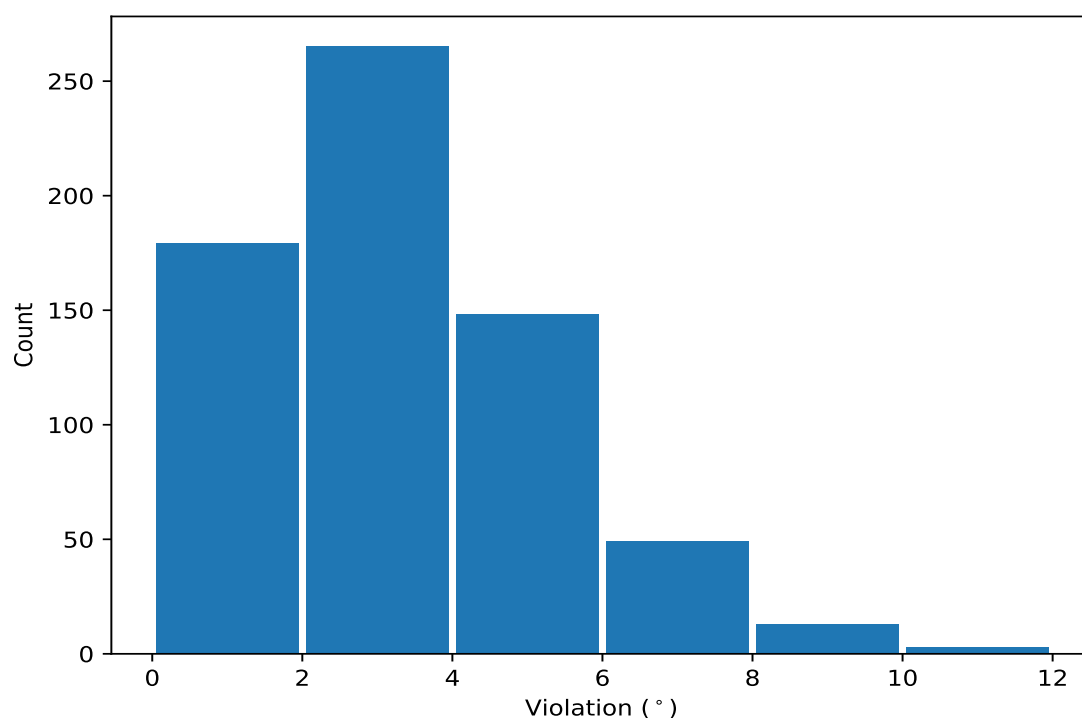
| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 19                  | 1.95 | 0.58            | 1.84   |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 18                  | 5.19 | 1.35            | 5.11   |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 18                  | 2.41 | 1.26            | 2.08   |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 18                  | 1.76 | 0.52            | 1.65   |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 18                  | 1.47 | 0.29            | 1.37   |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 17                  | 2.28 | 0.72            | 1.93   |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 17                  | 1.94 | 0.46            | 2.0    |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 16                  | 3.22 | 0.89            | 3.44   |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 14                  | 1.69 | 0.32            | 1.7    |
| (1,50) | 1:35:A:LEU:C | 1:36:A:THR:N  | 1:36:A:THR:CA | 1:36:A:THR:C | 12                  | 2.08 | 0.58            | 2.13   |
| (1,52) | 1:37:A:GLY:C | 1:38:A:VAL:N  | 1:38:A:VAL:CA | 1:38:A:VAL:C | 11                  | 2.78 | 0.88            | 3.05   |
| (1,7)  | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:ILE:N  | 11                  | 1.69 | 0.35            | 1.79   |
| (1,72) | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:PRO:N | 11                  | 1.28 | 0.18            | 1.25   |
| (1,8)  | 1:5:A:ILE:C  | 1:6:A:ILE:N   | 1:6:A:ILE:CA  | 1:6:A:ILE:C  | 10                  | 1.62 | 0.43            | 1.44   |
| (1,5)  | 1:4:A:PRO:N  | 1:4:A:PRO:CA  | 1:4:A:PRO:C   | 1:5:A:ILE:N  | 8                   | 1.26 | 0.19            | 1.21   |
| (1,64) | 1:45:A:LEU:N | 1:45:A:LEU:CA | 1:45:A:LEU:C  | 1:46:A:LEU:N | 7                   | 1.96 | 0.26            | 2.04   |
| (1,92) | 1:73:A:MET:N | 1:73:A:MET:CA | 1:73:A:MET:C  | 1:74:A:MET:N | 6                   | 1.86 | 0.48            | 1.77   |
| (1,84) | 1:67:A:LYS:N | 1:67:A:LYS:CA | 1:67:A:LYS:C  | 1:68:A:PRO:N | 6                   | 1.15 | 0.14            | 1.08   |
| (1,53) | 1:38:A:VAL:N | 1:38:A:VAL:CA | 1:38:A:VAL:C  | 1:39:A:LEU:N | 3                   | 3.34 | 0.48            | 3.42   |
| (1,63) | 1:44:A:LYS:C | 1:45:A:LEU:N  | 1:45:A:LEU:CA | 1:45:A:LEU:C | 3                   | 2.27 | 0.34            | 2.34   |
| (1,27) | 1:21:A:GLU:N | 1:21:A:GLU:CA | 1:21:A:GLU:C  | 1:22:A:ASP:N | 3                   | 1.46 | 0.23            | 1.33   |
| (1,26) | 1:20:A:SER:C | 1:21:A:GLU:N  | 1:21:A:GLU:CA | 1:21:A:GLU:C | 3                   | 1.26 | 0.04            | 1.28   |
| (1,73) | 1:58:A:ASP:C | 1:59:A:VAL:N  | 1:59:A:VAL:CA | 1:59:A:VAL:C | 3                   | 1.15 | 0.16            | 1.07   |
| (1,14) | 1:8:A:LYS:C  | 1:9:A:TRP:N   | 1:9:A:TRP:CA  | 1:9:A:TRP:C  | 2                   | 1.98 | 0.3             | 1.98   |

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

## 10.5 All violated dihedral-angle restraints ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 11       | 10.86         |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 17       | 10.44         |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 5        | 10.0          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 8        | 9.99          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 20       | 9.63          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 2        | 9.51          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 11       | 9.5           |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 1        | 9.34          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 17       | 9.05          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 6        | 8.8           |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 17       | 8.56          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 6        | 8.53          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 3        | 8.44          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 5        | 8.37          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 1        | 8.3           |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 1        | 8.28          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 8        | 7.94          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 3        | 7.89          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 11       | 7.77          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 2        | 7.74          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 2        | 7.62          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 3        | 7.56          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 16       | 7.53          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 6        | 7.51          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 8        | 7.45          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 5        | 7.38          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 16       | 7.36          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 11       | 7.27          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 6        | 7.2           |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 10       | 7.19          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 15       | 7.11          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 19       | 7.1           |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 7        | 7.1           |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 16       | 7.02          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 12       | 7.01          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 20       | 6.98          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 15       | 6.98          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 16       | 6.95          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 10       | 6.9           |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 13       | 6.89          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 13       | 6.8           |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 4        | 6.77          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 19       | 6.77          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 14       | 6.74          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 20       | 6.74          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 13       | 6.67          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 1        | 6.67          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 4        | 6.63          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 10       | 6.62          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 7        | 6.46          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 10       | 6.45          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 19       | 6.45          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 15       | 6.43          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 14       | 6.41          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 14       | 6.4           |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 14       | 6.37          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 7        | 6.36          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 17       | 6.26          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 20       | 6.24          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 20       | 6.24          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 10       | 6.24          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 14       | 6.24          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 16       | 6.17          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 19       | 6.15          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 19       | 6.05          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 8        | 5.96          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 12       | 5.94          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 5        | 5.93          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 18       | 5.92          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 15       | 5.91          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 4        | 5.81          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 9        | 5.8           |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 13       | 5.79          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 15       | 5.77          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 4        | 5.76          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 18       | 5.76          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 2        | 5.64          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 5        | 5.64          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 12       | 5.6           |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 6        | 5.56          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 9        | 5.54          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 13       | 5.53          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 18       | 5.51          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 8        | 5.38          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 3        | 5.37          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 11       | 5.33          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 19       | 5.33          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 20       | 5.32          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 3        | 5.32          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 1        | 5.32          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 3        | 5.29          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 15       | 5.28          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 9        | 5.24          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 13       | 5.23          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 3        | 5.22          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 12       | 5.22          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 16       | 5.21          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 11       | 5.21          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 8        | 5.17          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 7        | 5.16          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 18       | 5.16          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 14       | 5.16          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 16       | 5.15          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 18       | 5.15          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 4        | 5.14          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 7        | 5.12          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 19       | 5.1           |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 8        | 5.1           |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 4        | 5.08          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 15       | 5.07          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 1        | 5.05          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 10       | 5.05          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 15       | 5.04          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 16       | 5.03          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 7        | 5.02          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 5        | 5.02          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 9        | 5.01          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 1        | 5.0           |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 12       | 4.98          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 18       | 4.97          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 9        | 4.96          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 17       | 4.95          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 7        | 4.94          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 12       | 4.92          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 10       | 4.91          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 3        | 4.9           |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 19       | 4.88          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 2        | 4.86          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 17       | 4.85          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 7        | 4.84          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 13       | 4.84          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 18       | 4.83          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 16       | 4.83          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 20       | 4.81          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 5        | 4.79          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 4        | 4.77          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 11       | 4.76          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 2        | 4.73          |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 14       | 4.71          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 5        | 4.7           |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 13       | 4.68          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 14       | 4.67          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 17       | 4.66          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 8        | 4.64          |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 7        | 4.63          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 10       | 4.63          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 2        | 4.61          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 14       | 4.6           |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 9        | 4.54          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 12       | 4.52          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 8        | 4.51          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 20       | 4.51          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 8        | 4.51          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 2        | 4.5           |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 18       | 4.5           |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 20       | 4.5           |
| (1,83) | 1:66:A:LEU:C | 1:67:A:LYS:N  | 1:67:A:LYS:CA | 1:67:A:LYS:C | 18       | 4.49          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 17       | 4.49          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 6        | 4.48          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 6        | 4.47          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 4        | 4.45          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 1        | 4.44          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 6        | 4.42          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 9        | 4.41          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 12       | 4.41          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 5        | 4.4           |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 3        | 4.39          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 12       | 4.39          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 14       | 4.38          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 17       | 4.37          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 17       | 4.36          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 3        | 4.33          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 11       | 4.31          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 14       | 4.31          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 9        | 4.29          |
| (1,52) | 1:37:A:GLY:C | 1:38:A:VAL:N  | 1:38:A:VAL:CA | 1:38:A:VAL:C | 9        | 4.27          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 2        | 4.27          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 20       | 4.27          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 10       | 4.24          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 19       | 4.23          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 2        | 4.23          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 11       | 4.22          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 20       | 4.21          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 5        | 4.21          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 11       | 4.19          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 6        | 4.18          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 1        | 4.17          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 8        | 4.15          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 5        | 4.14          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 3        | 4.12          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 11       | 4.12          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 7        | 4.11          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 17       | 4.09          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 6        | 4.08          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 10       | 4.08          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 15       | 4.07          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 11       | 4.07          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 5        | 4.07          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 5        | 4.07          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 13       | 4.06          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 4        | 4.05          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 15       | 4.05          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 6        | 4.04          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 20       | 4.04          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 6        | 4.03          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 12       | 4.03          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 7        | 4.02          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 12       | 4.02          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 5        | 4.02          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 3        | 4.01          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 5        | 4.01          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 1        | 4.0           |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 9        | 4.0           |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 19       | 3.99          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 6        | 3.99          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 16       | 3.98          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 8        | 3.98          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 5        | 3.97          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 1        | 3.96          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 7        | 3.96          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 18       | 3.93          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 6        | 3.93          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 12       | 3.93          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 16       | 3.93          |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 4        | 3.92          |

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Continued from previous page...

| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 2        | 3.92          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 13       | 3.92          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 4        | 3.91          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 12       | 3.9           |
| (1,53) | 1:38:A:VAL:N | 1:38:A:VAL:CA | 1:38:A:VAL:C  | 1:39:A:LEU:N | 18       | 3.89          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 7        | 3.88          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 13       | 3.88          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 2        | 3.87          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 4        | 3.87          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 19       | 3.87          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 2        | 3.86          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 3        | 3.86          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 19       | 3.86          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 2        | 3.86          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 14       | 3.85          |
| (1,41) | 1:31:A:PHE:N | 1:31:A:PHE:CA | 1:31:A:PHE:C  | 1:32:A:LEU:N | 16       | 3.85          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 3        | 3.84          |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 18       | 3.83          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 4        | 3.83          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 9        | 3.83          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 4        | 3.83          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 14       | 3.82          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 17       | 3.82          |
| (1,60) | 1:42:A:ARG:N | 1:42:A:ARG:CA | 1:42:A:ARG:C  | 1:43:A:GLN:N | 9        | 3.81          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 13       | 3.81          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 8        | 3.8           |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 19       | 3.79          |
| (1,96) | 1:75:A:MET:N | 1:75:A:MET:CA | 1:75:A:MET:C  | 1:76:A:GLY:N | 11       | 3.78          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 5        | 3.78          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 11       | 3.77          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 8        | 3.77          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 3        | 3.77          |
| (1,52) | 1:37:A:GLY:C | 1:38:A:VAL:N  | 1:38:A:VAL:CA | 1:38:A:VAL:C | 14       | 3.76          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 10       | 3.76          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 2        | 3.76          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 1        | 3.74          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 11       | 3.73          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 4        | 3.7           |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 9        | 3.69          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 13       | 3.68          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 7        | 3.68          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 7        | 3.68          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 7        | 3.68          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 9        | 3.67          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 10       | 3.66          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 5        | 3.66          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 17       | 3.65          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 19       | 3.64          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 16       | 3.64          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 18       | 3.64          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 3        | 3.63          |

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*Continued from previous page...*

| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 16       | 3.63          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 18       | 3.63          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 2        | 3.63          |
| (1,56) | 1:40:A:PRO:N | 1:40:A:PRO:CA | 1:40:A:PRO:C  | 1:41:A:GLU:N | 9        | 3.62          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 16       | 3.62          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 10       | 3.62          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 15       | 3.62          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 3        | 3.61          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 12       | 3.61          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 8        | 3.6           |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 20       | 3.6           |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 15       | 3.59          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 15       | 3.59          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 1        | 3.57          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 20       | 3.56          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 17       | 3.56          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 14       | 3.56          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 12       | 3.55          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 4        | 3.54          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 16       | 3.54          |
| (1,52) | 1:37:A:GLY:C | 1:38:A:VAL:N  | 1:38:A:VAL:CA | 1:38:A:VAL:C | 18       | 3.53          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 17       | 3.52          |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 13       | 3.5           |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 15       | 3.5           |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 3        | 3.5           |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 3        | 3.5           |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 13       | 3.5           |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 11       | 3.5           |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 15       | 3.5           |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 1        | 3.5           |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 19       | 3.5           |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 20       | 3.49          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 15       | 3.49          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 13       | 3.48          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 1        | 3.48          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 2        | 3.47          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 20       | 3.46          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 1        | 3.46          |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 10       | 3.44          |
| (1,59) | 1:41:A:GLU:C | 1:42:A:ARG:N  | 1:42:A:ARG:CA | 1:42:A:ARG:C | 17       | 3.44          |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 12       | 3.43          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 5        | 3.43          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 14       | 3.43          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 4        | 3.43          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 15       | 3.42          |
| (1,53) | 1:38:A:VAL:N | 1:38:A:VAL:CA | 1:38:A:VAL:C  | 1:39:A:LEU:N | 9        | 3.42          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 20       | 3.41          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 4        | 3.41          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 6        | 3.41          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 8        | 3.4           |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 10       | 3.4           |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 14       | 3.39          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 7        | 3.39          |
| (1,47) | 1:34:A:THR:N | 1:34:A:THR:CA | 1:34:A:THR:C  | 1:35:A:LEU:N | 10       | 3.39          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 14       | 3.38          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 7        | 3.38          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 13       | 3.37          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 9        | 3.37          |
| (1,29) | 1:25:A:VAL:N | 1:25:A:VAL:CA | 1:25:A:VAL:C  | 1:26:A:LEU:N | 10       | 3.37          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 1        | 3.35          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 1        | 3.35          |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 14       | 3.34          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 15       | 3.33          |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 20       | 3.33          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 14       | 3.33          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 18       | 3.33          |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 16       | 3.32          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 17       | 3.3           |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 19       | 3.3           |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 19       | 3.3           |
| (1,81) | 1:63:A:ALA:C | 1:64:A:LEU:N  | 1:64:A:LEU:CA | 1:64:A:LEU:C | 8        | 3.29          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 9        | 3.27          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 15       | 3.26          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 12       | 3.26          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 6        | 3.25          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 18       | 3.25          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 2        | 3.25          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 16       | 3.25          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 18       | 3.25          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 6        | 3.24          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 7        | 3.23          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 12       | 3.22          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 15       | 3.17          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 1        | 3.16          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 16       | 3.16          |
| (1,52) | 1:37:A:GLY:C | 1:38:A:VAL:N  | 1:38:A:VAL:CA | 1:38:A:VAL:C | 12       | 3.15          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 16       | 3.14          |
| (1,50) | 1:35:A:LEU:C | 1:36:A:THR:N  | 1:36:A:THR:CA | 1:36:A:THR:C | 9        | 3.14          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 11       | 3.11          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 14       | 3.07          |
| (1,52) | 1:37:A:GLY:C | 1:38:A:VAL:N  | 1:38:A:VAL:CA | 1:38:A:VAL:C | 4        | 3.06          |
| (1,52) | 1:37:A:GLY:C | 1:38:A:VAL:N  | 1:38:A:VAL:CA | 1:38:A:VAL:C | 7        | 3.05          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 11       | 3.04          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 18       | 3.03          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 13       | 3.02          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 14       | 3.0           |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 9        | 3.0           |
| (1,50) | 1:35:A:LEU:C | 1:36:A:THR:N  | 1:36:A:THR:CA | 1:36:A:THR:C | 18       | 2.99          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 9        | 2.97          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 16       | 2.95          |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 13       | 2.95          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 8        | 2.92          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 10       | 2.92          |
| (1,51) | 1:36:A:THR:N | 1:36:A:THR:CA | 1:36:A:THR:C  | 1:37:A:GLY:N | 18       | 2.9           |
| (1,36) | 1:28:A:LEU:C | 1:29:A:LYS:N  | 1:29:A:LYS:CA | 1:29:A:LYS:C | 17       | 2.89          |
| (1,34) | 1:27:A:ASP:C | 1:28:A:LEU:N  | 1:28:A:LEU:CA | 1:28:A:LEU:C | 13       | 2.89          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 19       | 2.88          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 19       | 2.86          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 19       | 2.85          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 1        | 2.83          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 2        | 2.83          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 12       | 2.82          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 10       | 2.81          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 9        | 2.8           |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 7        | 2.77          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 12       | 2.77          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 18       | 2.77          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 18       | 2.75          |
| (1,32) | 1:26:A:LEU:C | 1:27:A:ASP:N  | 1:27:A:ASP:CA | 1:27:A:ASP:C | 6        | 2.75          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 20       | 2.75          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 7        | 2.74          |
| (1,53) | 1:38:A:VAL:N | 1:38:A:VAL:CA | 1:38:A:VAL:C  | 1:39:A:LEU:N | 20       | 2.72          |
| (1,92) | 1:73:A:MET:N | 1:73:A:MET:CA | 1:73:A:MET:C  | 1:74:A:MET:N | 17       | 2.71          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 4        | 2.68          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 4        | 2.65          |
| (1,63) | 1:44:A:LYS:C | 1:45:A:LEU:N  | 1:45:A:LEU:CA | 1:45:A:LEU:C | 18       | 2.64          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 1        | 2.64          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 12       | 2.61          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 6        | 2.61          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 19       | 2.61          |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 16       | 2.6           |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 15       | 2.6           |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 6        | 2.59          |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 20       | 2.59          |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 19       | 2.58          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 10       | 2.58          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 6        | 2.57          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 19       | 2.54          |
| (1,76) | 1:61:A:LEU:N | 1:61:A:LEU:CA | 1:61:A:LEU:C  | 1:62:A:GLY:N | 9        | 2.53          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 20       | 2.51          |
| (1,79) | 1:62:A:GLY:C | 1:63:A:ALA:N  | 1:63:A:ALA:CA | 1:63:A:ALA:C | 3        | 2.49          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 4        | 2.48          |
| (1,8)  | 1:5:A:ILE:C  | 1:6:A:ILE:N   | 1:6:A:ILE:CA  | 1:6:A:ILE:C  | 8        | 2.48          |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 14       | 2.46          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 14       | 2.44          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 18       | 2.43          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 19       | 2.39          |
| (1,43) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:LYS:N | 18       | 2.37          |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 17       | 2.35          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 8        | 2.35          |
| (1,63) | 1:44:A:LYS:C | 1:45:A:LEU:N  | 1:45:A:LEU:CA | 1:45:A:LEU:C | 20       | 2.34          |
| (1,52) | 1:37:A:GLY:C | 1:38:A:VAL:N  | 1:38:A:VAL:CA | 1:38:A:VAL:C | 15       | 2.34          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 8        | 2.32          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 13       | 2.32          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 17       | 2.32          |
| (1,52) | 1:37:A:GLY:C | 1:38:A:VAL:N  | 1:38:A:VAL:CA | 1:38:A:VAL:C | 16       | 2.31          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 16       | 2.3           |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 3        | 2.29          |
| (1,64) | 1:45:A:LEU:N | 1:45:A:LEU:CA | 1:45:A:LEU:C  | 1:46:A:LEU:N | 3        | 2.29          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 1        | 2.29          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 10       | 2.29          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 10       | 2.28          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 15       | 2.28          |
| (1,14) | 1:8:A:LYS:C  | 1:9:A:TRP:N   | 1:9:A:TRP:CA  | 1:9:A:TRP:C  | 1        | 2.28          |
| (1,7)  | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:ILE:N  | 16       | 2.28          |
| (1,50) | 1:35:A:LEU:C | 1:36:A:THR:N  | 1:36:A:THR:CA | 1:36:A:THR:C | 12       | 2.24          |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 18       | 2.23          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 17       | 2.22          |
| (1,82) | 1:64:A:LEU:N | 1:64:A:LEU:CA | 1:64:A:LEU:C  | 1:65:A:LYS:N | 11       | 2.21          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 7        | 2.21          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 10       | 2.21          |
| (1,50) | 1:35:A:LEU:C | 1:36:A:THR:N  | 1:36:A:THR:CA | 1:36:A:THR:C | 15       | 2.21          |
| (1,50) | 1:35:A:LEU:C | 1:36:A:THR:N  | 1:36:A:THR:CA | 1:36:A:THR:C | 7        | 2.18          |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 15       | 2.18          |
| (1,92) | 1:73:A:MET:N | 1:73:A:MET:CA | 1:73:A:MET:C  | 1:74:A:MET:N | 3        | 2.17          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 6        | 2.17          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 6        | 2.17          |
| (1,52) | 1:37:A:GLY:C | 1:38:A:VAL:N  | 1:38:A:VAL:CA | 1:38:A:VAL:C | 13       | 2.17          |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 18       | 2.16          |
| (1,50) | 1:35:A:LEU:C | 1:36:A:THR:N  | 1:36:A:THR:CA | 1:36:A:THR:C | 13       | 2.14          |
| (1,8)  | 1:5:A:ILE:C  | 1:6:A:ILE:N   | 1:6:A:ILE:CA  | 1:6:A:ILE:C  | 3        | 2.14          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 15       | 2.13          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 14       | 2.12          |
| (1,50) | 1:35:A:LEU:C | 1:36:A:THR:N  | 1:36:A:THR:CA | 1:36:A:THR:C | 4        | 2.12          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 6        | 2.09          |
| (1,64) | 1:45:A:LEU:N | 1:45:A:LEU:CA | 1:45:A:LEU:C  | 1:46:A:LEU:N | 16       | 2.09          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 16       | 2.09          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 11       | 2.08          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 16       | 2.06          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 4        | 2.06          |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 12       | 2.06          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 2        | 2.06          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 3        | 2.06          |
| (1,7)  | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:ILE:N  | 14       | 2.06          |
| (1,64) | 1:45:A:LEU:N | 1:45:A:LEU:CA | 1:45:A:LEU:C  | 1:46:A:LEU:N | 5        | 2.04          |
| (1,64) | 1:45:A:LEU:N | 1:45:A:LEU:CA | 1:45:A:LEU:C  | 1:46:A:LEU:N | 17       | 2.04          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 4        | 2.04          |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 13       | 2.03          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 13       | 2.02          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 12       | 2.0           |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 7        | 2.0           |
| (1,7)  | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:ILE:N  | 18       | 2.0           |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 2        | 1.99          |
| (1,50) | 1:35:A:LEU:C | 1:36:A:THR:N  | 1:36:A:THR:CA | 1:36:A:THR:C | 16       | 1.99          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 8        | 1.98          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 15       | 1.97          |
| (1,64) | 1:45:A:LEU:N | 1:45:A:LEU:CA | 1:45:A:LEU:C  | 1:46:A:LEU:N | 14       | 1.94          |
| (1,8)  | 1:5:A:ILE:C  | 1:6:A:ILE:N   | 1:6:A:ILE:CA  | 1:6:A:ILE:C  | 9        | 1.94          |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 5        | 1.93          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 13       | 1.93          |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 20       | 1.93          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 8        | 1.93          |
| (1,64) | 1:45:A:LEU:N | 1:45:A:LEU:CA | 1:45:A:LEU:C  | 1:46:A:LEU:N | 19       | 1.93          |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 9        | 1.93          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 16       | 1.93          |
| (1,50) | 1:35:A:LEU:C | 1:36:A:THR:N  | 1:36:A:THR:CA | 1:36:A:THR:C | 10       | 1.92          |
| (1,50) | 1:35:A:LEU:C | 1:36:A:THR:N  | 1:36:A:THR:CA | 1:36:A:THR:C | 14       | 1.92          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 1        | 1.9           |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 14       | 1.88          |
| (1,92) | 1:73:A:MET:N | 1:73:A:MET:CA | 1:73:A:MET:C  | 1:74:A:MET:N | 5        | 1.86          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 18       | 1.86          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 11       | 1.86          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 7        | 1.85          |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 4        | 1.85          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 2        | 1.84          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 12       | 1.84          |
| (1,7)  | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:ILE:N  | 15       | 1.84          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 7        | 1.83          |
| (1,63) | 1:44:A:LYS:C | 1:45:A:LEU:N  | 1:45:A:LEU:CA | 1:45:A:LEU:C | 9        | 1.82          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 5        | 1.81          |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 10       | 1.81          |
| (1,8)  | 1:5:A:ILE:C  | 1:6:A:ILE:N   | 1:6:A:ILE:CA  | 1:6:A:ILE:C  | 5        | 1.81          |
| (1,7)  | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:ILE:N  | 2        | 1.8           |
| (1,54) | 1:38:A:VAL:C | 1:39:A:LEU:N  | 1:39:A:LEU:CA | 1:39:A:LEU:C | 9        | 1.79          |
| (1,7)  | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:ILE:N  | 6        | 1.79          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 17       | 1.78          |
| (1,27) | 1:21:A:GLU:N | 1:21:A:GLU:CA | 1:21:A:GLU:C  | 1:22:A:ASP:N | 7        | 1.78          |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 9        | 1.77          |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 8        | 1.76          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 11       | 1.76          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 11       | 1.75          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 13       | 1.74          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 1        | 1.73          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 11       | 1.72          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 10       | 1.71          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 12       | 1.71          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 2        | 1.71          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 15       | 1.71          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 4        | 1.7           |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 9        | 1.7           |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 6        | 1.7           |
| (1,92) | 1:73:A:MET:N | 1:73:A:MET:CA | 1:73:A:MET:C  | 1:74:A:MET:N | 6        | 1.68          |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 1        | 1.68          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 12       | 1.68          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 19       | 1.68          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,14) | 1:8:A:LYS:C  | 1:9:A:TRP:N   | 1:9:A:TRP:CA  | 1:9:A:TRP:C  | 8        | 1.68          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 4        | 1.67          |
| (1,52) | 1:37:A:GLY:C | 1:38:A:VAL:N  | 1:38:A:VAL:CA | 1:38:A:VAL:C | 10       | 1.67          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 8        | 1.64          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 19       | 1.64          |
| (1,7)  | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:ILE:N  | 11       | 1.64          |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 11       | 1.63          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 17       | 1.63          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 17       | 1.61          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 5        | 1.6           |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 10       | 1.6           |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 4        | 1.59          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 13       | 1.59          |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 14       | 1.59          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 5        | 1.59          |
| (1,5)  | 1:4:A:PRO:N  | 1:4:A:PRO:CA  | 1:4:A:PRO:C   | 1:5:A:ILE:N  | 14       | 1.58          |
| (1,72) | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:PRO:N | 20       | 1.57          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 4        | 1.57          |
| (1,5)  | 1:4:A:PRO:N  | 1:4:A:PRO:CA  | 1:4:A:PRO:C   | 1:5:A:ILE:N  | 13       | 1.57          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 2        | 1.56          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 7        | 1.56          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 18       | 1.54          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 7        | 1.54          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 3        | 1.53          |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 3        | 1.53          |
| (1,8)  | 1:5:A:ILE:C  | 1:6:A:ILE:N   | 1:6:A:ILE:CA  | 1:6:A:ILE:C  | 1        | 1.53          |
| (1,7)  | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:ILE:N  | 4        | 1.53          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 14       | 1.51          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 10       | 1.51          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 13       | 1.51          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 15       | 1.5           |
| (1,72) | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:PRO:N | 19       | 1.5           |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 5        | 1.5           |
| (1,92) | 1:73:A:MET:N | 1:73:A:MET:CA | 1:73:A:MET:C  | 1:74:A:MET:N | 8        | 1.48          |
| (1,72) | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:PRO:N | 2        | 1.48          |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 18       | 1.46          |
| (1,97) | 1:76:A:GLY:C | 1:77:A:THR:N  | 1:77:A:THR:CA | 1:77:A:THR:C | 11       | 1.45          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 13       | 1.45          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 3        | 1.45          |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 7        | 1.43          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 20       | 1.43          |
| (1,93) | 1:73:A:MET:C | 1:74:A:MET:N  | 1:74:A:MET:CA | 1:74:A:MET:C | 19       | 1.42          |
| (1,72) | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:PRO:N | 9        | 1.42          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 11       | 1.41          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 16       | 1.4           |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 10       | 1.39          |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 12       | 1.39          |
| (1,64) | 1:45:A:LEU:N | 1:45:A:LEU:CA | 1:45:A:LEU:C  | 1:46:A:LEU:N | 15       | 1.39          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 16       | 1.38          |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 12       | 1.38          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 12       | 1.37          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 14       | 1.37          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 17       | 1.37          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 20       | 1.37          |
| (1,73) | 1:58:A:ASP:C | 1:59:A:VAL:N  | 1:59:A:VAL:CA | 1:59:A:VAL:C | 8        | 1.37          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 17       | 1.37          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 7        | 1.35          |
| (1,84) | 1:67:A:LYS:N | 1:67:A:LYS:CA | 1:67:A:LYS:C  | 1:68:A:PRO:N | 2        | 1.35          |
| (1,84) | 1:67:A:LYS:N | 1:67:A:LYS:CA | 1:67:A:LYS:C  | 1:68:A:PRO:N | 18       | 1.35          |
| (1,8)  | 1:5:A:ILE:C  | 1:6:A:ILE:N   | 1:6:A:ILE:CA  | 1:6:A:ILE:C  | 6        | 1.35          |
| (1,8)  | 1:5:A:ILE:C  | 1:6:A:ILE:N   | 1:6:A:ILE:CA  | 1:6:A:ILE:C  | 17       | 1.34          |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 4        | 1.33          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 19       | 1.33          |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 16       | 1.33          |
| (1,27) | 1:21:A:GLU:N | 1:21:A:GLU:CA | 1:21:A:GLU:C  | 1:22:A:ASP:N | 13       | 1.33          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 6        | 1.32          |
| (1,31) | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 6        | 1.32          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 5        | 1.3           |
| (1,55) | 1:39:A:LEU:N | 1:39:A:LEU:CA | 1:39:A:LEU:C  | 1:40:A:PRO:N | 5        | 1.3           |
| (1,26) | 1:20:A:SER:C | 1:21:A:GLU:N  | 1:21:A:GLU:CA | 1:21:A:GLU:C | 2        | 1.3           |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 8        | 1.29          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 20       | 1.29          |
| (1,61) | 1:43:A:GLN:C | 1:44:A:LYS:N  | 1:44:A:LYS:CA | 1:44:A:LYS:C | 20       | 1.29          |
| (1,7)  | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:ILE:N  | 13       | 1.29          |
| (1,26) | 1:20:A:SER:C | 1:21:A:GLU:N  | 1:21:A:GLU:CA | 1:21:A:GLU:C | 16       | 1.28          |
| (1,72) | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:PRO:N | 18       | 1.27          |
| (1,27) | 1:21:A:GLU:N | 1:21:A:GLU:CA | 1:21:A:GLU:C  | 1:22:A:ASP:N | 8        | 1.27          |
| (1,5)  | 1:4:A:PRO:N  | 1:4:A:PRO:CA  | 1:4:A:PRO:C   | 1:5:A:ILE:N  | 6        | 1.27          |
| (1,8)  | 1:5:A:ILE:C  | 1:6:A:ILE:N   | 1:6:A:ILE:CA  | 1:6:A:ILE:C  | 10       | 1.26          |
| (1,72) | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:PRO:N | 10       | 1.25          |
| (1,5)  | 1:4:A:PRO:N  | 1:4:A:PRO:CA  | 1:4:A:PRO:C   | 1:5:A:ILE:N  | 15       | 1.25          |
| (1,92) | 1:73:A:MET:N | 1:73:A:MET:CA | 1:73:A:MET:C  | 1:74:A:MET:N | 1        | 1.24          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 15       | 1.24          |
| (1,8)  | 1:5:A:ILE:C  | 1:6:A:ILE:N   | 1:6:A:ILE:CA  | 1:6:A:ILE:C  | 7        | 1.24          |
| (1,52) | 1:37:A:GLY:C | 1:38:A:VAL:N  | 1:38:A:VAL:CA | 1:38:A:VAL:C | 19       | 1.23          |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 20       | 1.23          |
| (1,11) | 1:7:A:VAL:N  | 1:7:A:VAL:CA  | 1:7:A:VAL:C   | 1:8:A:LYS:N  | 14       | 1.23          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 3        | 1.22          |
| (1,78) | 1:62:A:GLY:N | 1:62:A:GLY:CA | 1:62:A:GLY:C  | 1:63:A:ALA:N | 9        | 1.22          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 14       | 1.22          |
| (1,86) | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 10       | 1.21          |
| (1,26) | 1:20:A:SER:C | 1:21:A:GLU:N  | 1:21:A:GLU:CA | 1:21:A:GLU:C | 13       | 1.21          |
| (1,90) | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 5        | 1.19          |
| (1,72) | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:PRO:N | 4        | 1.19          |
| (1,49) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C  | 1:36:A:THR:N | 19       | 1.18          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 3        | 1.18          |
| (1,7)  | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:ILE:N  | 19       | 1.18          |
| (1,72) | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:PRO:N | 17       | 1.17          |
| (1,38) | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 8        | 1.17          |
| (1,5)  | 1:4:A:PRO:N  | 1:4:A:PRO:CA  | 1:4:A:PRO:C   | 1:5:A:ILE:N  | 18       | 1.17          |
| (1,62) | 1:44:A:LYS:N | 1:44:A:LYS:CA | 1:44:A:LYS:C  | 1:45:A:LEU:N | 3        | 1.16          |
| (1,7)  | 1:5:A:ILE:N  | 1:5:A:ILE:CA  | 1:5:A:ILE:C   | 1:6:A:ILE:N  | 9        | 1.15          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,100) | 1:78:A:ARG:N | 1:78:A:ARG:CA | 1:78:A:ARG:C  | 1:79:A:GLU:N | 20       | 1.12          |
| (1,84)  | 1:67:A:LYS:N | 1:67:A:LYS:CA | 1:67:A:LYS:C  | 1:68:A:PRO:N | 1        | 1.11          |
| (1,31)  | 1:26:A:LEU:N | 1:26:A:LEU:CA | 1:26:A:LEU:C  | 1:27:A:ASP:N | 2        | 1.11          |
| (1,5)   | 1:4:A:PRO:N  | 1:4:A:PRO:CA  | 1:4:A:PRO:C   | 1:5:A:ILE:N  | 17       | 1.11          |
| (1,72)  | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:PRO:N | 11       | 1.1           |
| (1,50)  | 1:35:A:LEU:C | 1:36:A:THR:N  | 1:36:A:THR:CA | 1:36:A:THR:C | 5        | 1.1           |
| (1,72)  | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:PRO:N | 7        | 1.09          |
| (1,38)  | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 9        | 1.09          |
| (1,38)  | 1:29:A:LYS:C | 1:30:A:GLN:N  | 1:30:A:GLN:CA | 1:30:A:GLN:C | 5        | 1.08          |
| (1,5)   | 1:4:A:PRO:N  | 1:4:A:PRO:CA  | 1:4:A:PRO:C   | 1:5:A:ILE:N  | 3        | 1.08          |
| (1,5)   | 1:4:A:PRO:N  | 1:4:A:PRO:CA  | 1:4:A:PRO:C   | 1:5:A:ILE:N  | 16       | 1.08          |
| (1,73)  | 1:58:A:ASP:C | 1:59:A:VAL:N  | 1:59:A:VAL:CA | 1:59:A:VAL:C | 3        | 1.07          |
| (1,16)  | 1:11:A:GLY:C | 1:12:A:GLN:N  | 1:12:A:GLN:CA | 1:12:A:GLN:C | 19       | 1.07          |
| (1,8)   | 1:5:A:ILE:C  | 1:6:A:ILE:N   | 1:6:A:ILE:CA  | 1:6:A:ILE:C  | 12       | 1.07          |
| (1,90)  | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 13       | 1.06          |
| (1,84)  | 1:67:A:LYS:N | 1:67:A:LYS:CA | 1:67:A:LYS:C  | 1:68:A:PRO:N | 11       | 1.06          |
| (1,50)  | 1:35:A:LEU:C | 1:36:A:THR:N  | 1:36:A:THR:CA | 1:36:A:THR:C | 19       | 1.05          |
| (1,72)  | 1:53:A:LYS:N | 1:53:A:LYS:CA | 1:53:A:LYS:C  | 1:54:A:PRO:N | 13       | 1.04          |
| (1,86)  | 1:69:A:ASN:N | 1:69:A:ASN:CA | 1:69:A:ASN:C  | 1:70:A:THR:N | 2        | 1.03          |
| (1,84)  | 1:67:A:LYS:N | 1:67:A:LYS:CA | 1:67:A:LYS:C  | 1:68:A:PRO:N | 17       | 1.03          |
| (1,90)  | 1:72:A:ILE:N | 1:72:A:ILE:CA | 1:72:A:ILE:C  | 1:73:A:MET:N | 6        | 1.02          |
| (1,89)  | 1:71:A:LYS:C | 1:72:A:ILE:N  | 1:72:A:ILE:CA | 1:72:A:ILE:C | 20       | 1.02          |
| (1,84)  | 1:67:A:LYS:N | 1:67:A:LYS:CA | 1:67:A:LYS:C  | 1:68:A:PRO:N | 5        | 1.01          |
| (1,73)  | 1:58:A:ASP:C | 1:59:A:VAL:N  | 1:59:A:VAL:CA | 1:59:A:VAL:C | 1        | 1.0           |