



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 2, 2026 – 02:11 AM UTC

PDB ID : 6ALK / pdb\_00006alk  
BMRB ID : 25590  
Title : NMR solution structure of the major beech pollen allergen Fag s 1  
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Deposited on : 2017-08-08

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

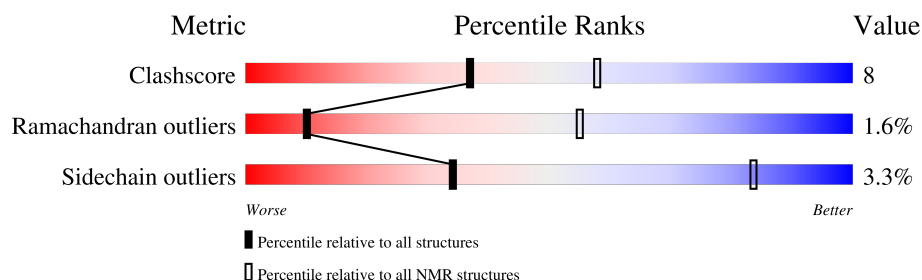
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 91%.

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     | 159    | <br>80% 13% • 7% |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                            |                   |              |
|--------------------------------------|----------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)      | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:2-A:59, A:65-A:154 (148) | 0.99              | 16           |

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 2433 atoms, of which 1216 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fag s 1 pollen allergen.

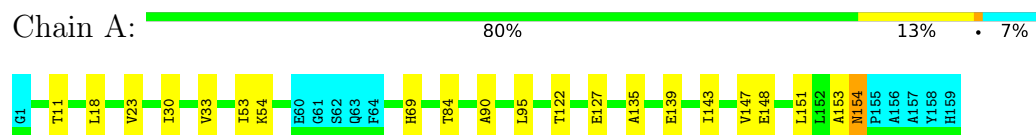
| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 159      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2433  | 776 | 1216 | 196 | 244 | 1 |       |

## 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: Fag s 1 pollen allergen

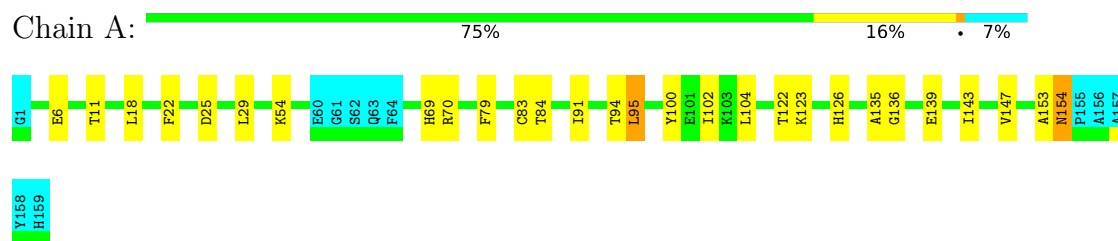


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

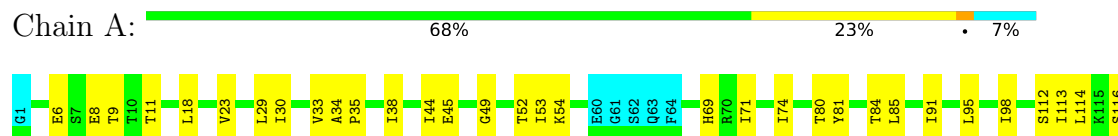
#### 4.2.1 Score per residue for model 1

- Molecule 1: Fag s 1 pollen allergen



#### 4.2.2 Score per residue for model 2

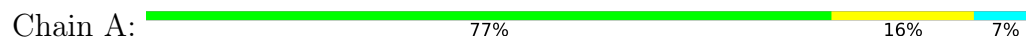
- Molecule 1: Fag s 1 pollen allergen





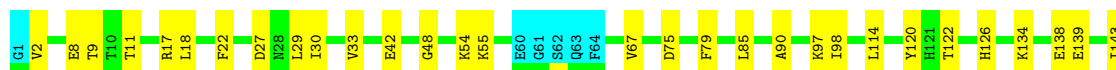
### 4.2.3 Score per residue for model 3

- Molecule 1: Fag s 1 pollen allergen



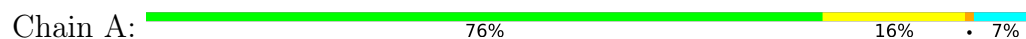
### 4.2.4 Score per residue for model 4

- Molecule 1: Fag s 1 pollen allergen



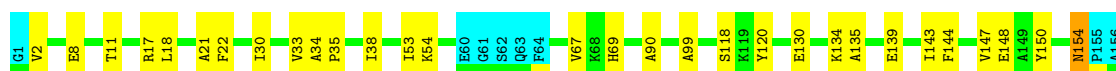
### 4.2.5 Score per residue for model 5

- Molecule 1: Fag s 1 pollen allergen



### 4.2.6 Score per residue for model 6

- Molecule 1: Fag s 1 pollen allergen

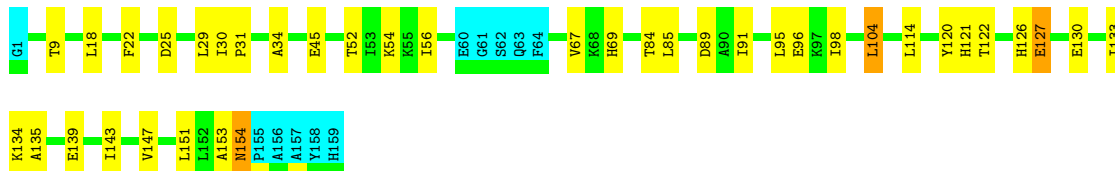




#### 4.2.7 Score per residue for model 7

- Molecule 1: Fag s 1 pollen allergen

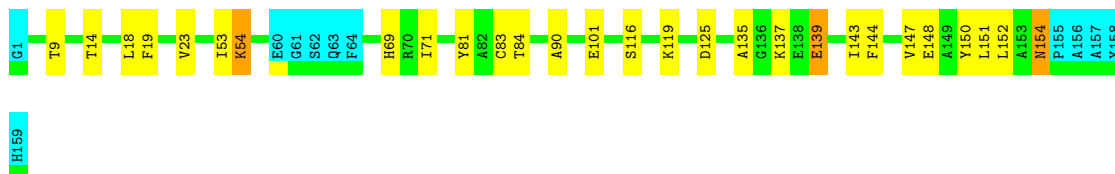
Chain A: 69% 22% 7%



#### 4.2.8 Score per residue for model 8

- Molecule 1: Fag s 1 pollen allergen

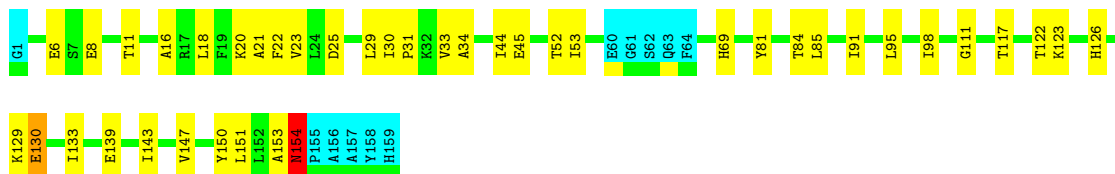
Chain A: 75% 16% 7%



#### 4.2.9 Score per residue for model 9

- Molecule 1: Fag s 1 pollen allergen

Chain A: 67% 25% 7%



#### 4.2.10 Score per residue for model 10

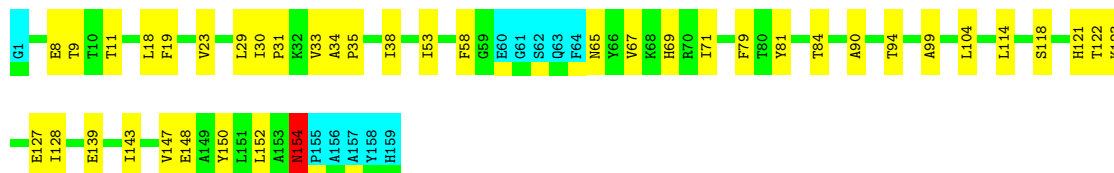
- Molecule 1: Fag s 1 pollen allergen

Chain A: 77% 16% 7%



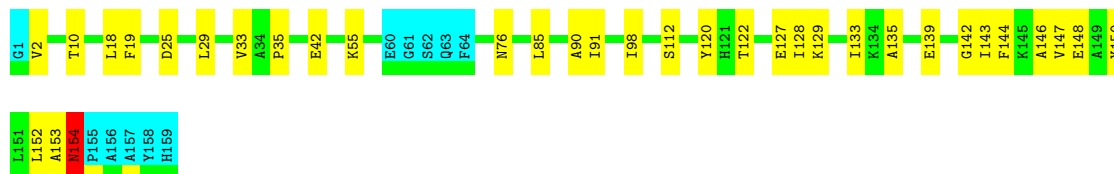
#### 4.2.11 Score per residue for model 11

- Molecule 1: Fag s 1 pollen allergen



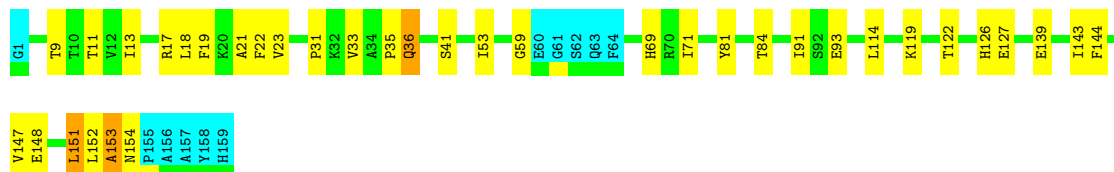
#### 4.2.12 Score per residue for model 12

- Molecule 1: Fag s 1 pollen allergen



#### 4.2.13 Score per residue for model 13

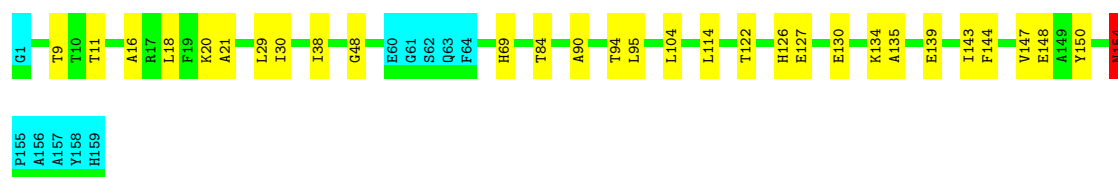
- Molecule 1: Fag s 1 pollen allergen



#### 4.2.14 Score per residue for model 14

- Molecule 1: Fag s 1 pollen allergen

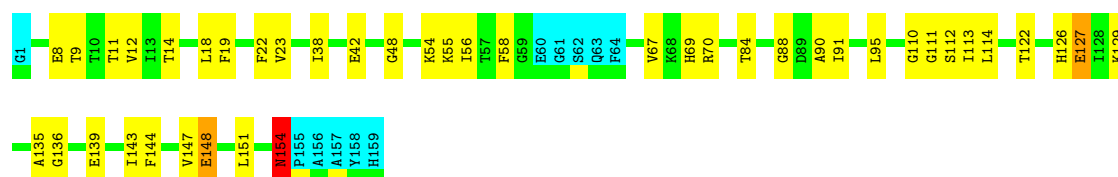




#### 4.2.15 Score per residue for model 15

- Molecule 1: Fag s 1 pollen allergen

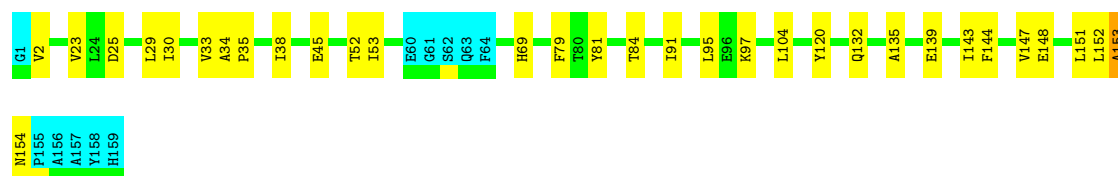
Chain A: 67% 25% 7%



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

- Molecule 1: Fag s 1 pollen allergen

Chain A: 73% 19% 7%



#### 4.2.17 Score per residue for model 17

- Molecule 1: Fag s 1 pollen allergen

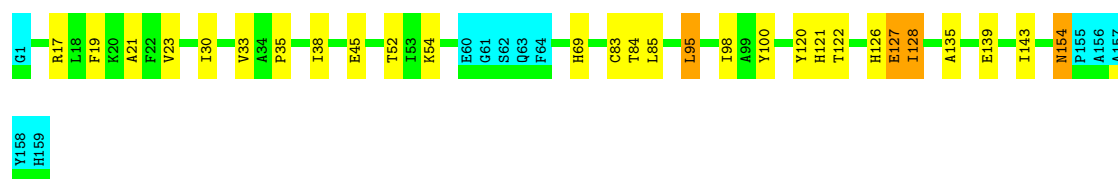
Chain A: 74% 19% 7%



#### 4.2.18 Score per residue for model 18

- Molecule 1: Fag s 1 pollen allergen

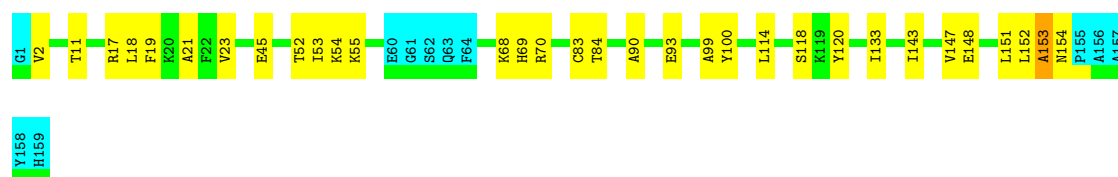
Chain A: 75% 15% 7%



#### 4.2.19 Score per residue for model 19

- Molecule 1: Fag s 1 pollen allergen

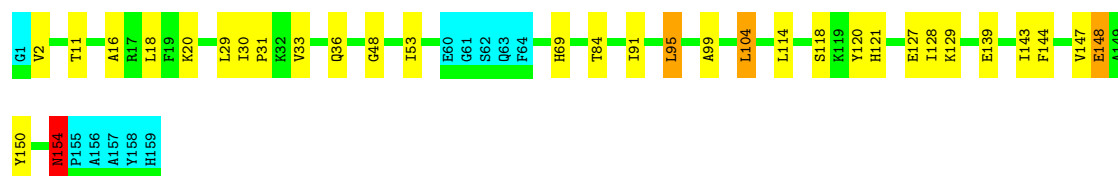
Chain A: 73% 19% 7%



#### 4.2.20 Score per residue for model 20

- Molecule 1: Fag s 1 pollen allergen

Chain A: 73% 18% 7%



## 5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| ARIA          | structure calculation | 2.3.1   |
| CNS           | structure calculation | 1.3.1   |

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                       | 1878           |
| Number of shifts mapped to atoms             | 1878           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 91%            |

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                       | Bond angles |                       |
|-----|-------|--------------|-----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                  | RMSZ        | #Z>5                  |
| 1   | A     | 0.45±0.01    | 0±0/1154 ( 0.0± 0.0%) | 0.71±0.02   | 0±0/1562 ( 0.0± 0.0%) |
| All | All   | 0.45         | 0/23080 ( 0.0%)       | 0.71        | 1/31240 ( 0.0%)       |

There are no bond-length outliers.

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 1   | A     | 127 | GLU  | CB-CA-C | -5.15 | 109.14      | 116.34   | 2      | 1     |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 1134  | 1146     | 1143     | 17±4    |
| All | All   | 22680 | 22920    | 22860    | 344     |

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 8.

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

| Atom-1          | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|-----------------|----------------|----------|-------------|--------|-------|
|                 |                |          |             | Worst  | Total |
| 1:A:23:VAL:HG13 | 1:A:81:TYR:CD2 | 0.65     | 2.27        | 13     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:139:GLU:O   | 1:A:143:ILE:HG12 | 0.65     | 1.92        | 4      | 6     |
| 1:A:135:ALA:O   | 1:A:139:GLU:HB2  | 0.63     | 1.92        | 8      | 11    |
| 1:A:148:GLU:O   | 1:A:152:LEU:HG   | 0.61     | 1.95        | 10     | 4     |
| 1:A:147:VAL:O   | 1:A:151:LEU:HG   | 0.61     | 1.95        | 8      | 7     |
| 1:A:69:HIS:HA   | 1:A:84:THR:O     | 0.60     | 1.95        | 15     | 17    |
| 1:A:18:LEU:O    | 1:A:22:PHE:HB3   | 0.60     | 1.97        | 9      | 7     |
| 1:A:99:ALA:O    | 1:A:118:SER:HA   | 0.60     | 1.96        | 19     | 5     |
| 1:A:104:LEU:HG  | 1:A:114:LEU:HD23 | 0.60     | 1.73        | 20     | 3     |
| 1:A:143:ILE:O   | 1:A:147:VAL:HG23 | 0.59     | 1.98        | 8      | 3     |
| 1:A:150:TYR:O   | 1:A:154:ASN:HB2  | 0.59     | 1.98        | 20     | 5     |
| 1:A:143:ILE:O   | 1:A:147:VAL:HG22 | 0.58     | 1.98        | 15     | 16    |
| 1:A:139:GLU:O   | 1:A:143:ILE:HG13 | 0.58     | 1.99        | 14     | 8     |
| 1:A:85:LEU:O    | 1:A:85:LEU:HD12  | 0.57     | 1.99        | 5      | 2     |
| 1:A:91:ILE:HG23 | 1:A:95:LEU:HB2   | 0.56     | 1.77        | 2      | 5     |
| 1:A:11:THR:OG1  | 1:A:18:LEU:HD11  | 0.56     | 2.00        | 13     | 11    |
| 1:A:33:VAL:C    | 1:A:35:PRO:HD3   | 0.56     | 2.25        | 3      | 9     |
| 1:A:130:GLU:O   | 1:A:134:LYS:HG2  | 0.55     | 2.01        | 6      | 3     |
| 1:A:95:LEU:HD22 | 1:A:127:GLU:O    | 0.55     | 2.01        | 2      | 3     |
| 1:A:45:GLU:O    | 1:A:52:THR:HA    | 0.54     | 2.03        | 19     | 7     |
| 1:A:71:ILE:HD11 | 1:A:81:TYR:CZ    | 0.54     | 2.38        | 8      | 2     |
| 1:A:11:THR:O    | 1:A:111:GLY:HA3  | 0.53     | 2.04        | 3      | 4     |
| 1:A:23:VAL:HG13 | 1:A:81:TYR:CD1   | 0.53     | 2.39        | 5      | 1     |
| 1:A:95:LEU:HD22 | 1:A:128:ILE:HA   | 0.53     | 1.80        | 17     | 2     |
| 1:A:19:PHE:O    | 1:A:23:VAL:HB    | 0.53     | 2.03        | 8      | 8     |
| 1:A:33:VAL:HG11 | 1:A:150:TYR:CG   | 0.53     | 2.39        | 4      | 1     |
| 1:A:18:LEU:HD13 | 1:A:114:LEU:HD11 | 0.53     | 1.79        | 5      | 1     |
| 1:A:35:PRO:O    | 1:A:59:GLY:HA3   | 0.53     | 2.04        | 13     | 1     |
| 1:A:56:ILE:HB   | 1:A:67:VAL:O     | 0.52     | 2.04        | 7      | 1     |
| 1:A:11:THR:HA   | 1:A:148:GLU:OE2  | 0.52     | 2.05        | 14     | 2     |
| 1:A:17:ARG:O    | 1:A:21:ALA:HB3   | 0.52     | 2.05        | 10     | 5     |
| 1:A:96:GLU:HB3  | 1:A:121:HIS:O    | 0.52     | 2.05        | 7      | 1     |
| 1:A:25:ASP:O    | 1:A:29:LEU:HG    | 0.52     | 2.05        | 9      | 5     |
| 1:A:122:THR:HB  | 1:A:126:HIS:O    | 0.51     | 2.04        | 1      | 9     |
| 1:A:83:CYS:SG   | 1:A:100:TYR:HB2  | 0.51     | 2.45        | 18     | 2     |
| 1:A:34:ALA:N    | 1:A:35:PRO:HD3   | 0.51     | 2.20        | 6      | 6     |
| 1:A:150:TYR:HA  | 1:A:154:ASN:CG   | 0.51     | 2.31        | 12     | 1     |
| 1:A:144:PHE:O   | 1:A:148:GLU:HB2  | 0.51     | 2.06        | 16     | 1     |
| 1:A:8:GLU:HA    | 1:A:114:LEU:O    | 0.50     | 2.05        | 15     | 3     |
| 1:A:42:GLU:HA   | 1:A:55:LYS:O     | 0.50     | 2.06        | 15     | 1     |
| 1:A:30:ILE:HA   | 1:A:34:ALA:HB3   | 0.50     | 1.82        | 7      | 2     |
| 1:A:121:HIS:O   | 1:A:128:ILE:HD11 | 0.50     | 2.05        | 20     | 3     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:101:GLU:O   | 1:A:116:SER:HA   | 0.49     | 2.07        | 8      | 1     |
| 1:A:112:SER:C   | 1:A:113:ILE:HG13 | 0.49     | 2.32        | 15     | 2     |
| 1:A:144:PHE:O   | 1:A:148:GLU:HB3  | 0.49     | 2.07        | 12     | 8     |
| 1:A:54:LYS:HE3  | 1:A:83:CYS:SG    | 0.49     | 2.48        | 17     | 2     |
| 1:A:12:VAL:HA   | 1:A:110:GLY:O    | 0.49     | 2.08        | 15     | 1     |
| 1:A:33:VAL:HG11 | 1:A:150:TYR:CD2  | 0.49     | 2.42        | 9      | 1     |
| 1:A:23:VAL:HG13 | 1:A:81:TYR:CE1   | 0.49     | 2.43        | 5      | 2     |
| 1:A:11:THR:HA   | 1:A:148:GLU:OE1  | 0.49     | 2.07        | 19     | 1     |
| 1:A:127:GLU:H   | 1:A:127:GLU:CD   | 0.49     | 2.14        | 18     | 3     |
| 1:A:91:ILE:CG2  | 1:A:95:LEU:HB2   | 0.49     | 2.38        | 1      | 1     |
| 1:A:27:ASP:OD2  | 1:A:42:GLU:HA    | 0.49     | 2.08        | 4      | 1     |
| 1:A:98:ILE:HG13 | 1:A:98:ILE:O     | 0.49     | 2.08        | 12     | 2     |
| 1:A:2:VAL:HA    | 1:A:120:TYR:O    | 0.49     | 2.08        | 19     | 6     |
| 1:A:30:ILE:CG2  | 1:A:38:ILE:HB    | 0.48     | 2.38        | 16     | 6     |
| 1:A:130:GLU:H   | 1:A:130:GLU:CD   | 0.48     | 2.15        | 9      | 1     |
| 1:A:23:VAL:HG13 | 1:A:81:TYR:CE2   | 0.48     | 2.44        | 16     | 2     |
| 1:A:42:GLU:HB2  | 1:A:55:LYS:CG    | 0.47     | 2.38        | 5      | 3     |
| 1:A:70:ARG:O    | 1:A:83:CYS:HA    | 0.47     | 2.09        | 1      | 1     |
| 1:A:16:ALA:O    | 1:A:20:LYS:HG2   | 0.47     | 2.09        | 14     | 3     |
| 1:A:120:TYR:CE1 | 1:A:133:ILE:HA   | 0.47     | 2.45        | 7      | 1     |
| 1:A:30:ILE:HB   | 1:A:31:PRO:HD3   | 0.47     | 1.87        | 7      | 5     |
| 1:A:151:LEU:C   | 1:A:153:ALA:H    | 0.47     | 2.17        | 19     | 4     |
| 1:A:135:ALA:HA  | 1:A:139:GLU:OE1  | 0.47     | 2.09        | 8      | 1     |
| 1:A:129:LYS:O   | 1:A:133:ILE:HG13 | 0.47     | 2.10        | 9      | 1     |
| 1:A:9:THR:HB    | 1:A:114:LEU:HB2  | 0.47     | 1.85        | 14     | 3     |
| 1:A:42:GLU:O    | 1:A:54:LYS:HG2   | 0.47     | 2.10        | 15     | 1     |
| 1:A:49:GLY:O    | 1:A:71:ILE:HB    | 0.46     | 2.10        | 5      | 2     |
| 1:A:95:LEU:C    | 1:A:123:LYS:HB2  | 0.46     | 2.35        | 9      | 1     |
| 1:A:10:THR:HA   | 1:A:112:SER:O    | 0.46     | 2.10        | 12     | 1     |
| 1:A:85:LEU:HD11 | 1:A:98:ILE:HG12  | 0.46     | 1.86        | 9      | 4     |
| 1:A:75:ASP:O    | 1:A:79:PHE:HA    | 0.46     | 2.11        | 4      | 1     |
| 1:A:9:THR:HB    | 1:A:114:LEU:HD12 | 0.46     | 1.88        | 11     | 3     |
| 1:A:85:LEU:CD2  | 1:A:91:ILE:HG13  | 0.45     | 2.41        | 12     | 1     |
| 1:A:85:LEU:HD12 | 1:A:85:LEU:C     | 0.45     | 2.37        | 5      | 1     |
| 1:A:18:LEU:HD22 | 1:A:18:LEU:N     | 0.45     | 2.26        | 12     | 2     |
| 1:A:38:ILE:HD13 | 1:A:56:ILE:HD12  | 0.45     | 1.87        | 15     | 1     |
| 1:A:6:GLU:HA    | 1:A:116:SER:O    | 0.45     | 2.11        | 2      | 1     |
| 1:A:33:VAL:HG11 | 1:A:150:TYR:CD1  | 0.45     | 2.47        | 11     | 1     |
| 1:A:42:GLU:HB2  | 1:A:54:LYS:HB3   | 0.45     | 1.89        | 15     | 1     |
| 1:A:151:LEU:C   | 1:A:153:ALA:N    | 0.45     | 2.75        | 2      | 4     |
| 1:A:30:ILE:HG21 | 1:A:38:ILE:HB    | 0.44     | 1.89        | 3      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:128:ILE:O    | 1:A:128:ILE:HG22 | 0.44     | 2.12        | 12     | 1     |
| 1:A:152:LEU:O    | 1:A:153:ALA:HB3  | 0.44     | 2.12        | 16     | 3     |
| 1:A:29:LEU:O     | 1:A:33:VAL:HG22  | 0.44     | 2.12        | 20     | 4     |
| 1:A:122:THR:CG2  | 1:A:127:GLU:HA   | 0.44     | 2.43        | 11     | 5     |
| 1:A:6:GLU:HB3    | 1:A:117:THR:HA   | 0.44     | 1.89        | 9      | 1     |
| 1:A:54:LYS:HB2   | 1:A:69:HIS:C     | 0.44     | 2.37        | 15     | 1     |
| 1:A:122:THR:OG1  | 1:A:126:HIS:HB2  | 0.43     | 2.13        | 15     | 1     |
| 1:A:79:PHE:CB    | 1:A:104:LEU:HB2  | 0.43     | 2.44        | 16     | 2     |
| 1:A:67:VAL:HG13  | 1:A:69:HIS:CE1   | 0.43     | 2.49        | 6      | 1     |
| 1:A:18:LEU:HD13  | 1:A:114:LEU:HD21 | 0.43     | 1.90        | 19     | 1     |
| 1:A:79:PHE:O     | 1:A:104:LEU:HB2  | 0.42     | 2.14        | 1      | 1     |
| 1:A:94:THR:C     | 1:A:95:LEU:HD12  | 0.42     | 2.38        | 14     | 1     |
| 1:A:135:ALA:O    | 1:A:139:GLU:HB3  | 0.42     | 2.14        | 14     | 2     |
| 1:A:136:GLY:HA2  | 1:A:139:GLU:OE2  | 0.42     | 2.13        | 15     | 1     |
| 1:A:94:THR:O     | 1:A:123:LYS:HB3  | 0.42     | 2.14        | 11     | 2     |
| 1:A:21:ALA:HB1   | 1:A:29:LEU:HD11  | 0.42     | 1.91        | 14     | 1     |
| 1:A:142:GLY:O    | 1:A:146:ALA:HB3  | 0.42     | 2.14        | 12     | 1     |
| 1:A:100:TYR:OH   | 1:A:136:GLY:HA2  | 0.42     | 2.14        | 1      | 1     |
| 1:A:19:PHE:CZ    | 1:A:76:ASN:HA    | 0.42     | 2.50        | 12     | 1     |
| 1:A:141:SER:HA   | 1:A:144:PHE:CE2  | 0.42     | 2.50        | 5      | 1     |
| 1:A:98:ILE:HG22  | 1:A:120:TYR:CD2  | 0.42     | 2.50        | 18     | 1     |
| 1:A:22:PHE:CD1   | 1:A:22:PHE:C     | 0.42     | 2.98        | 13     | 1     |
| 1:A:74:ILE:HA    | 1:A:80:THR:O     | 0.41     | 2.14        | 2      | 1     |
| 1:A:20:LYS:HG3   | 1:A:21:ALA:N     | 0.41     | 2.29        | 9      | 1     |
| 1:A:44:ILE:HB    | 1:A:53:ILE:HB    | 0.41     | 1.91        | 9      | 2     |
| 1:A:154:ASN:N    | 1:A:154:ASN:HD22 | 0.41     | 2.14        | 13     | 1     |
| 1:A:22:PHE:C     | 1:A:22:PHE:CD2   | 0.41     | 2.98        | 4      | 1     |
| 1:A:31:PRO:HG3   | 1:A:41:SER:H     | 0.41     | 1.76        | 13     | 1     |
| 1:A:36:GLN:HE21  | 1:A:36:GLN:HA    | 0.41     | 1.75        | 13     | 1     |
| 1:A:67:VAL:HB    | 1:A:90:ALA:HB3   | 0.41     | 1.92        | 4      | 1     |
| 1:A:56:ILE:HG13  | 1:A:69:HIS:CE1   | 0.41     | 2.51        | 15     | 1     |
| 1:A:67:VAL:HA    | 1:A:88:GLY:HA3   | 0.41     | 1.92        | 15     | 1     |
| 1:A:102:ILE:HD12 | 1:A:102:ILE:N    | 0.41     | 2.31        | 1      | 1     |
| 1:A:20:LYS:O     | 1:A:24:LEU:HB3   | 0.41     | 2.16        | 10     | 1     |
| 1:A:54:LYS:HD3   | 1:A:70:ARG:CA    | 0.41     | 2.45        | 15     | 1     |
| 1:A:9:THR:HG22   | 1:A:11:THR:CG2   | 0.41     | 2.46        | 5      | 1     |
| 1:A:68:LYS:HB2   | 1:A:87:GLU:O     | 0.41     | 2.15        | 10     | 1     |
| 1:A:102:ILE:CG2  | 1:A:114:LEU:HB3  | 0.41     | 2.46        | 5      | 1     |
| 1:A:30:ILE:H     | 1:A:30:ILE:HD12  | 0.41     | 1.76        | 4      | 1     |
| 1:A:55:LYS:HA    | 1:A:68:LYS:HA    | 0.40     | 1.93        | 19     | 1     |
| 1:A:85:LEU:HD22  | 1:A:98:ILE:O     | 0.40     | 2.16        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:71:ILE:HD12 | 1:A:81:TYR:CE2  | 0.40     | 2.51        | 13     | 1     |
| 1:A:15:PRO:HA   | 1:A:18:LEU:HD23 | 0.40     | 1.94        | 3      | 1     |
| 1:A:134:LYS:O   | 1:A:138:GLU:HG2 | 0.40     | 2.16        | 4      | 1     |
| 1:A:22:PHE:CD2  | 1:A:22:PHE:C    | 0.40     | 2.99        | 6      | 1     |
| 1:A:9:THR:HB    | 1:A:114:LEU:CD1 | 0.40     | 2.46        | 15     | 1     |
| 1:A:30:ILE:HG22 | 1:A:38:ILE:HB   | 0.40     | 1.94        | 11     | 1     |

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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

| Mol | Chain | Analysed        | Favoured      | Allowed      | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|--------------|------------|-------------|----|
| 1   | A     | 148/159 (93%)   | 128±3 (86±2%) | 18±3 (12±2%) | 2±1 (2±1%) | 10          | 55 |
| All | All   | 2960/3180 (93%) | 2557 (86%)    | 356 (12%)    | 47 (2%)    | 10          | 55 |

All 9 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     | 154 | ASN  | 16             |
| 1   | A     | 90  | ALA  | 10             |
| 1   | A     | 153 | ALA  | 6              |
| 1   | A     | 48  | GLY  | 5              |
| 1   | A     | 93  | GLU  | 3              |
| 1   | A     | 129 | LYS  | 3              |
| 1   | A     | 65  | ASN  | 2              |
| 1   | A     | 89  | ASP  | 1              |
| 1   | A     | 128 | ILE  | 1              |

### 6.3.2 Protein sidechains

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

| Mol | Chain | Analysed        | Rotameric     | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|------------|-------------|----|
| 1   | A     | 122/129 (95%)   | 118±2 (97±2%) | 4±2 (3±2%) | 34          | 83 |
| All | All   | 2440/2580 (95%) | 2360 (97%)    | 80 (3%)    | 34          | 83 |

All 29 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     | 154 | ASN  | 10             |
| 1   | A     | 54  | LYS  | 9              |
| 1   | A     | 53  | ILE  | 9              |
| 1   | A     | 127 | GLU  | 7              |
| 1   | A     | 8   | GLU  | 4              |
| 1   | A     | 95  | LEU  | 3              |
| 1   | A     | 148 | GLU  | 3              |
| 1   | A     | 152 | LEU  | 3              |
| 1   | A     | 133 | ILE  | 3              |
| 1   | A     | 119 | LYS  | 3              |
| 1   | A     | 97  | LYS  | 2              |
| 1   | A     | 9   | THR  | 2              |
| 1   | A     | 104 | LEU  | 2              |
| 1   | A     | 14  | THR  | 2              |
| 1   | A     | 91  | ILE  | 2              |
| 1   | A     | 151 | LEU  | 2              |
| 1   | A     | 36  | GLN  | 2              |
| 1   | A     | 6   | GLU  | 1              |
| 1   | A     | 125 | ASP  | 1              |
| 1   | A     | 137 | LYS  | 1              |
| 1   | A     | 139 | GLU  | 1              |
| 1   | A     | 130 | GLU  | 1              |
| 1   | A     | 25  | ASP  | 1              |
| 1   | A     | 67  | VAL  | 1              |
| 1   | A     | 13  | ILE  | 1              |
| 1   | A     | 93  | GLU  | 1              |
| 1   | A     | 132 | GLN  | 1              |
| 1   | A     | 94  | THR  | 1              |
| 1   | A     | 70  | ARG  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 90% 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                  | 1878 |
| Number of shifts mapped to atoms        | 1878 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 0    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 155      | $-0.39 \pm 0.17$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 144      | $0.10 \pm 0.15$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 144      | $0.03 \pm 0.10$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 140      | $0.89 \pm 0.43$                 | Should be applied          |

#### 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 91%, i.e. 1786 atoms were assigned a chemical shift out of a possible 1958. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|---------------|-----------------|-----------------|
| Backbone  | 703/741 (95%)   | 289/302 (96%) | 282/296 (95%)   | 132/143 (92%)   |
| Sidechain | 1006/1079 (93%) | 687/704 (98%) | 310/347 (89%)   | 9/28 (32%)      |

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|          | Total           | <sup>1</sup> H  | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|-----------------|-----------------|-----------------|
| Aromatic | 77/138 (56%)    | 49/66 (74%)     | 28/66 (42%)     | 0/6 (0%)        |
| Overall  | 1786/1958 (91%) | 1025/1072 (96%) | 620/709 (87%)   | 141/177 (80%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1878 atoms were assigned a chemical shift out of a possible 2086. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H  | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone  | 747/796 (94%)   | 308/325 (95%)   | 299/318 (94%)   | 140/153 (92%)   |
| Sidechain | 1047/1125 (93%) | 715/734 (97%)   | 322/362 (89%)   | 10/29 (34%)     |
| Aromatic  | 84/165 (51%)    | 53/79 (67%)     | 31/78 (40%)     | 0/8 (0%)        |
| Overall   | 1878/2086 (90%) | 1076/1138 (95%) | 652/758 (86%)   | 150/190 (79%)   |

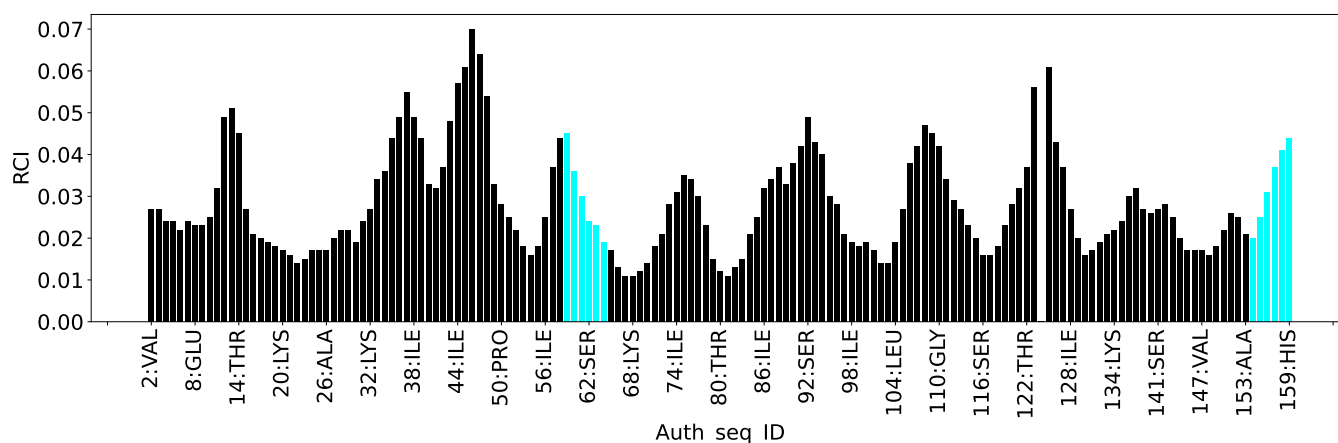
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 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                                | 2046  |
| Intra-residue ( $ i-j =0$ )                              | 712   |
| Sequential ( $ i-j =1$ )                                 | 507   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 246   |
| Long range ( $ i-j \geq 5$ )                             | 501   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 80    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 177   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 14.0  |
| Number of long range restraints per residue <sup>1</sup> | 3.5   |

<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)  | 36.8                                   | 0.2     |
| 0.2-0.5 (Medium) | 62.4                                   | 0.5     |
| >0.5 (Large)     | 84.1                                   | 3.9     |

### 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)   | 8.1                                    | 7.09    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

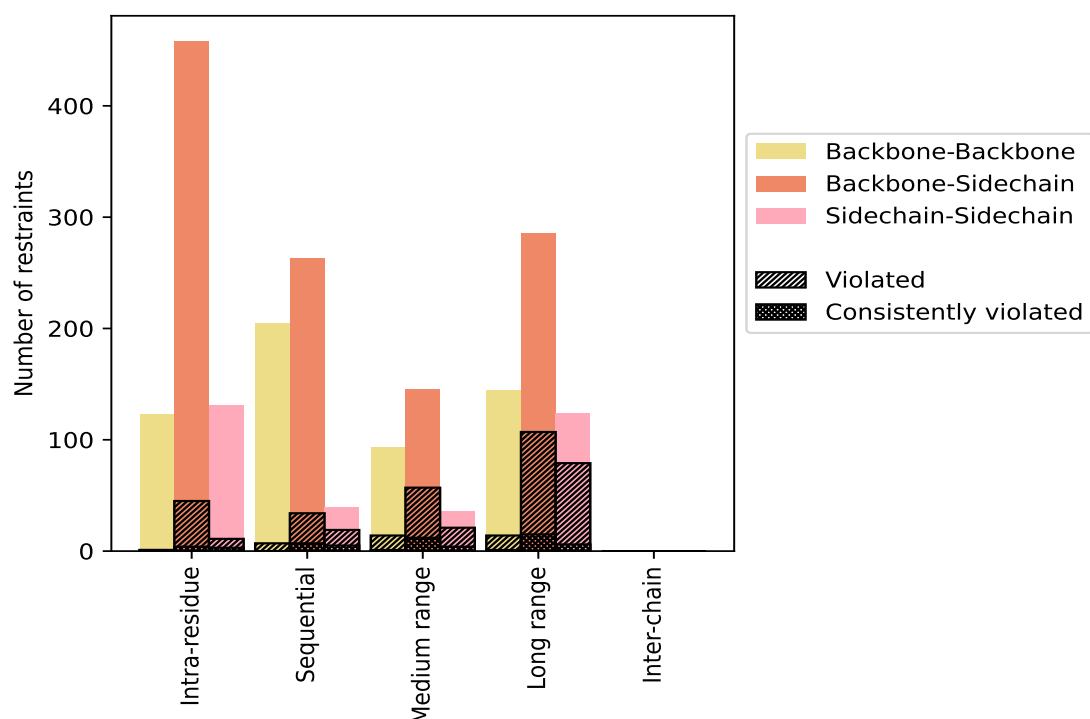
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>712</b>  | <b>34.8</b>    | <b>57</b>             | <b>8.0</b>     | <b>2.8</b>     | <b>8</b>                           | <b>1.1</b>     | <b>0.4</b>     |
| Backbone-Backbone                                                           | 123         | 6.0            | 1                     | 0.8            | 0.0            | 1                                  | 0.8            | 0.0            |
| Backbone-Sidechain                                                          | 458         | 22.4           | 45                    | 9.8            | 2.2            | 4                                  | 0.9            | 0.2            |
| Sidechain-Sidechain                                                         | 131         | 6.4            | 11                    | 8.4            | 0.5            | 3                                  | 2.3            | 0.1            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>507</b>  | <b>24.8</b>    | <b>60</b>             | <b>11.8</b>    | <b>2.9</b>     | <b>12</b>                          | <b>2.4</b>     | <b>0.6</b>     |
| Backbone-Backbone                                                           | 205         | 10.0           | 7                     | 3.4            | 0.3            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 263         | 12.9           | 34                    | 12.9           | 1.7            | 7                                  | 2.7            | 0.3            |
| Sidechain-Sidechain                                                         | 39          | 1.9            | 19                    | 48.7           | 0.9            | 5                                  | 12.8           | 0.2            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>246</b>  | <b>12.0</b>    | <b>87</b>             | <b>35.4</b>    | <b>4.3</b>     | <b>17</b>                          | <b>6.9</b>     | <b>0.8</b>     |
| Backbone-Backbone                                                           | 93          | 4.5            | 14                    | 15.1           | 0.7            | 1                                  | 1.1            | 0.0            |
| Backbone-Sidechain                                                          | 117         | 5.7            | 52                    | 44.4           | 2.5            | 12                                 | 10.3           | 0.6            |
| Sidechain-Sidechain                                                         | 36          | 1.8            | 21                    | 58.3           | 1.0            | 4                                  | 11.1           | 0.2            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>501</b>  | <b>24.5</b>    | <b>192</b>            | <b>38.3</b>    | <b>9.4</b>     | <b>22</b>                          | <b>4.4</b>     | <b>1.1</b>     |
| Backbone-Backbone                                                           | 144         | 7.0            | 14                    | 9.7            | 0.7            | 1                                  | 0.7            | 0.0            |
| Backbone-Sidechain                                                          | 233         | 11.4           | 99                    | 42.5           | 4.8            | 15                                 | 6.4            | 0.7            |
| Sidechain-Sidechain                                                         | 124         | 6.1            | 79                    | 63.7           | 3.9            | 6                                  | 4.8            | 0.3            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>80</b>   | <b>3.9</b>     | <b>13</b>             | <b>16.2</b>    | <b>0.6</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>2046</b> | <b>100.0</b>   | <b>409</b>            | <b>20.0</b>    | <b>20.0</b>    | <b>59</b>                          | <b>2.9</b>     | <b>2.9</b>     |
| Backbone-Backbone                                                           | 565         | 27.6           | 36                    | 6.4            | 1.8            | 3                                  | 0.5            | 0.1            |
| Backbone-Sidechain                                                          | 1151        | 56.3           | 243                   | 21.1           | 11.9           | 38                                 | 3.3            | 1.9            |
| Sidechain-Sidechain                                                         | 330         | 16.1           | 130                   | 39.4           | 6.4            | 18                                 | 5.5            | 0.9            |

<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        | 24                   | 31              | 45              | 85              | 0               | 185   | 0.6      | 2.44    | 0.49                | 0.45       |
| 2        | 22                   | 35              | 48              | 81              | 0               | 186   | 0.66     | 3.26    | 0.59                | 0.5        |
| 3        | 28                   | 38              | 52              | 83              | 0               | 201   | 0.68     | 3.04    | 0.57                | 0.5        |
| 4        | 26                   | 36              | 46              | 82              | 0               | 190   | 0.67     | 3.39    | 0.55                | 0.48       |
| 5        | 27                   | 31              | 44              | 87              | 0               | 189   | 0.65     | 2.65    | 0.54                | 0.46       |
| 6        | 24                   | 32              | 43              | 87              | 0               | 186   | 0.62     | 3.07    | 0.51                | 0.46       |
| 7        | 22                   | 30              | 41              | 95              | 0               | 188   | 0.58     | 2.8     | 0.49                | 0.42       |
| 8        | 21                   | 35              | 46              | 87              | 0               | 189   | 0.62     | 2.93    | 0.54                | 0.46       |
| 9        | 24                   | 30              | 48              | 83              | 0               | 185   | 0.67     | 2.85    | 0.54                | 0.51       |
| 10       | 23                   | 33              | 44              | 86              | 0               | 186   | 0.59     | 2.47    | 0.48                | 0.45       |

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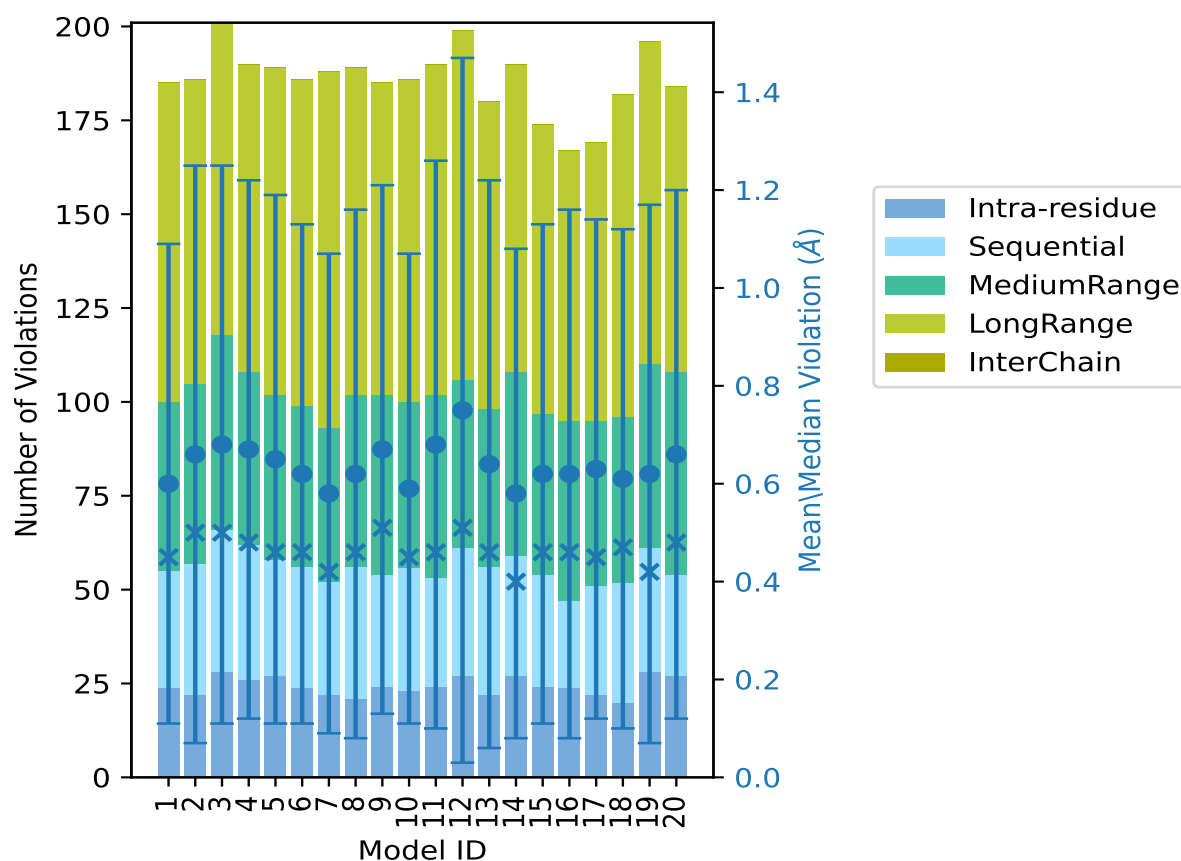
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 24                   | 29              | 49              | 88              | 0               | 190   | 0.68     | 2.56    | 0.58                | 0.46       |
| 12       | 27                   | 34              | 45              | 93              | 0               | 199   | 0.75     | 3.55    | 0.72                | 0.51       |
| 13       | 22                   | 34              | 42              | 82              | 0               | 180   | 0.64     | 3.9     | 0.58                | 0.46       |
| 14       | 27                   | 32              | 49              | 82              | 0               | 190   | 0.58     | 3.23    | 0.5                 | 0.4        |
| 15       | 24                   | 30              | 43              | 77              | 0               | 174   | 0.62     | 2.42    | 0.51                | 0.46       |
| 16       | 24                   | 23              | 48              | 72              | 0               | 167   | 0.62     | 3.06    | 0.54                | 0.46       |
| 17       | 22                   | 29              | 44              | 74              | 0               | 169   | 0.63     | 2.67    | 0.51                | 0.45       |
| 18       | 20                   | 32              | 44              | 86              | 0               | 182   | 0.61     | 2.9     | 0.51                | 0.47       |
| 19       | 28                   | 33              | 49              | 86              | 0               | 196   | 0.62     | 3.11    | 0.55                | 0.42       |
| 20       | 27                   | 27              | 54              | 76              | 0               | 184   | 0.66     | 3.24    | 0.54                | 0.48       |

<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

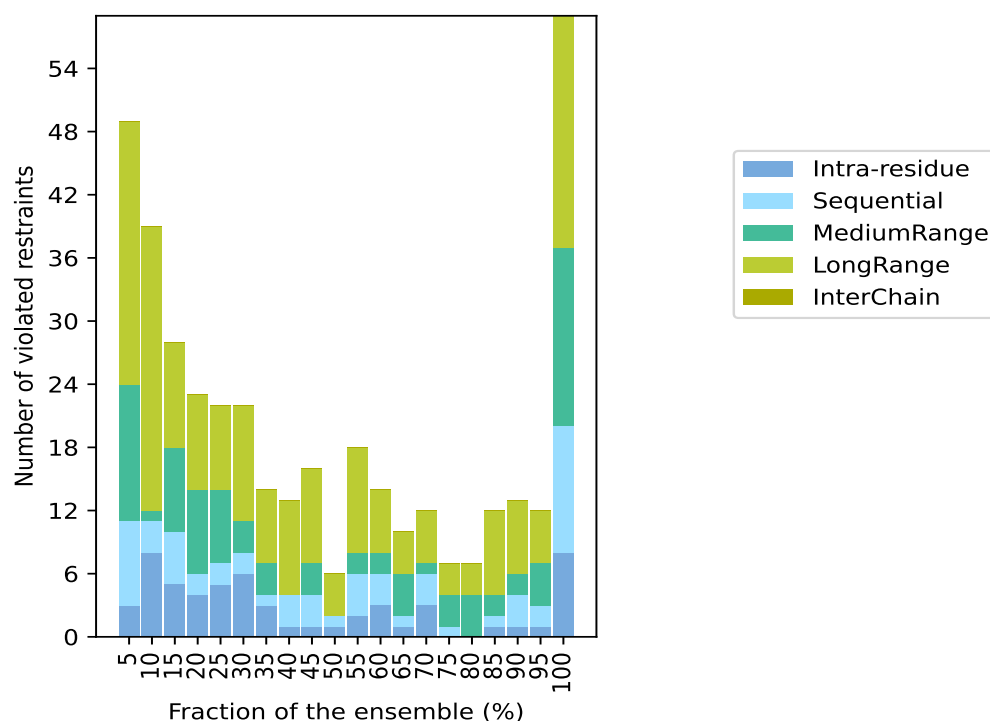
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1570(IR:655, SQ:447, MR:159, LR:309, IC:0) restraints are 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>       | %     |
| 3                             | 8               | 13              | 25              | 0               | 49    | 1                        | 5.0   |
| 8                             | 3               | 1               | 27              | 0               | 39    | 2                        | 10.0  |
| 5                             | 5               | 8               | 10              | 0               | 28    | 3                        | 15.0  |
| 4                             | 2               | 8               | 9               | 0               | 23    | 4                        | 20.0  |
| 5                             | 2               | 7               | 8               | 0               | 22    | 5                        | 25.0  |
| 6                             | 2               | 3               | 11              | 0               | 22    | 6                        | 30.0  |
| 3                             | 1               | 3               | 7               | 0               | 14    | 7                        | 35.0  |
| 1                             | 3               | 0               | 9               | 0               | 13    | 8                        | 40.0  |
| 1                             | 3               | 3               | 9               | 0               | 16    | 9                        | 45.0  |
| 1                             | 1               | 0               | 4               | 0               | 6     | 10                       | 50.0  |
| 2                             | 4               | 2               | 10              | 0               | 18    | 11                       | 55.0  |
| 3                             | 3               | 2               | 6               | 0               | 14    | 12                       | 60.0  |
| 1                             | 1               | 4               | 4               | 0               | 10    | 13                       | 65.0  |
| 3                             | 3               | 1               | 5               | 0               | 12    | 14                       | 70.0  |
| 0                             | 1               | 3               | 3               | 0               | 7     | 15                       | 75.0  |
| 0                             | 0               | 4               | 3               | 0               | 7     | 16                       | 80.0  |
| 1                             | 1               | 2               | 8               | 0               | 12    | 17                       | 85.0  |
| 1                             | 3               | 2               | 7               | 0               | 13    | 18                       | 90.0  |
| 1                             | 2               | 4               | 5               | 0               | 12    | 19                       | 95.0  |
| 8                             | 12              | 17              | 22              | 0               | 59    | 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

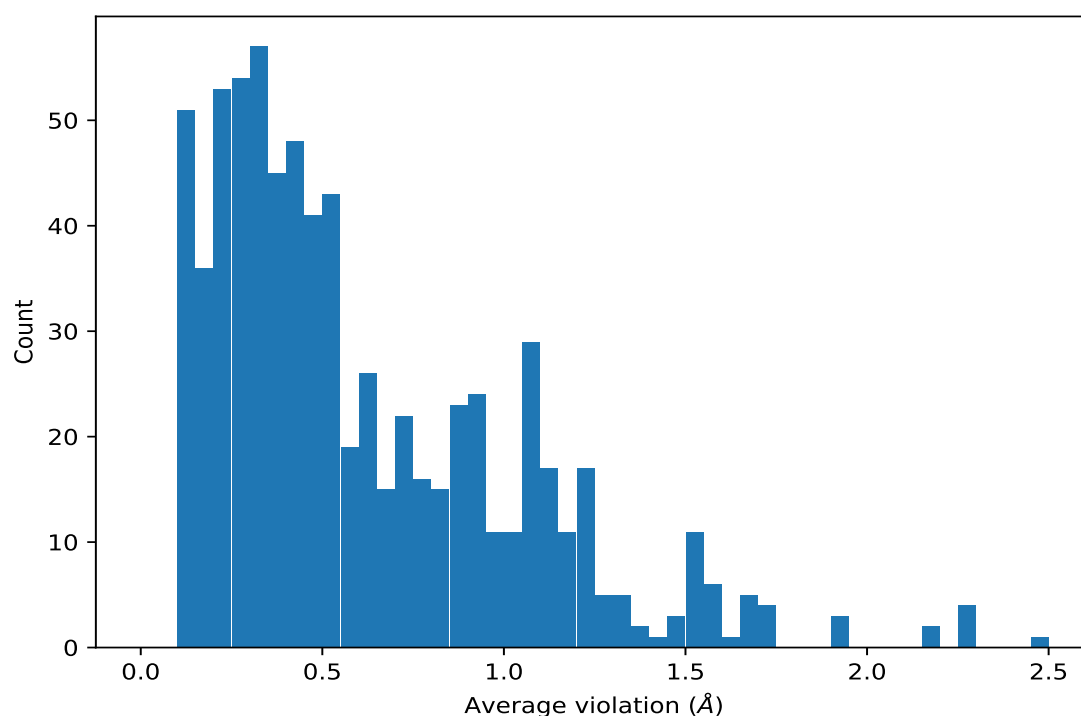
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1071) | 1:23:A:VAL:HG12 | 1:22:A:PHE:HB3  | 20                  | 2.28     | 0.13                | 2.26       |
| (1,1071) | 1:23:A:VAL:HG11 | 1:22:A:PHE:HB3  | 20                  | 2.28     | 0.13                | 2.26       |
| (1,1071) | 1:23:A:VAL:HG13 | 1:22:A:PHE:HB3  | 20                  | 2.28     | 0.13                | 2.26       |
| (1,1562) | 1:145:A:LYS:HB2 | 1:142:A:GLY:HA3 | 20                  | 2.26     | 0.53                | 2.54       |
| (1,1148) | 1:31:A:PRO:HG3  | 1:27:A:ASP:HB3  | 20                  | 1.72     | 0.36                | 1.83       |
| (1,1546) | 1:153:A:ALA:HB2 | 1:152:A:LEU:HA  | 20                  | 1.68     | 0.74                | 1.91       |
| (1,1546) | 1:153:A:ALA:HB1 | 1:152:A:LEU:HA  | 20                  | 1.68     | 0.74                | 1.91       |
| (1,1546) | 1:153:A:ALA:HB3 | 1:152:A:LEU:HA  | 20                  | 1.68     | 0.74                | 1.91       |
| (1,1680) | 1:149:A:ALA:HA  | 1:151:A:LEU:HB3 | 20                  | 1.6      | 0.13                | 1.65       |
| (1,1630) | 1:121:A:HIS:HB3 | 1:91:A:ILE:HD12 | 20                  | 1.52     | 0.24                | 1.56       |
| (1,1630) | 1:121:A:HIS:HB3 | 1:91:A:ILE:HD11 | 20                  | 1.52     | 0.24                | 1.56       |
| (1,1630) | 1:121:A:HIS:HB3 | 1:91:A:ILE:HD13 | 20                  | 1.52     | 0.24                | 1.56       |
| (3,72)   | 1:11:A:THR:HG22 | 1:15:A:PRO:HA   | 20                  | 1.5      | 0.28                | 1.54       |
| (3,72)   | 1:11:A:THR:HG21 | 1:15:A:PRO:HA   | 20                  | 1.5      | 0.28                | 1.54       |
| (3,72)   | 1:11:A:THR:HG23 | 1:15:A:PRO:HA   | 20                  | 1.5      | 0.28                | 1.54       |
| (1,1010) | 1:31:A:PRO:HD2  | 1:41:A:SER:HA   | 20                  | 1.37     | 0.19                | 1.43       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG21  | 20                  | 1.25     | 0.23                | 1.17       |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG22  | 20                  | 1.25     | 0.23                | 1.17       |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG23  | 20                  | 1.25     | 0.23                | 1.17       |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 20                  | 1.24     | 0.13                | 1.24       |
| (1,1019) | 1:146:A:ALA:HB1  | 1:142:A:GLY:HA3  | 20                  | 1.24     | 0.07                | 1.23       |
| (1,1019) | 1:146:A:ALA:HB2  | 1:142:A:GLY:HA3  | 20                  | 1.24     | 0.07                | 1.23       |
| (1,1019) | 1:146:A:ALA:HB3  | 1:142:A:GLY:HA3  | 20                  | 1.24     | 0.07                | 1.23       |
| (1,1701) | 1:153:A:ALA:HB1  | 1:154:A:ASN:HD22 | 20                  | 1.18     | 0.61                | 1.05       |
| (1,1701) | 1:153:A:ALA:HB3  | 1:154:A:ASN:HD22 | 20                  | 1.18     | 0.61                | 1.05       |
| (1,1701) | 1:153:A:ALA:HB2  | 1:154:A:ASN:HD22 | 20                  | 1.18     | 0.61                | 1.05       |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 20                  | 1.15     | 0.18                | 1.21       |
| (1,1573) | 1:113:A:ILE:HD13 | 1:106:A:ALA:HB1  | 20                  | 1.13     | 0.08                | 1.12       |
| (1,1573) | 1:113:A:ILE:HD13 | 1:106:A:ALA:HB3  | 20                  | 1.13     | 0.08                | 1.12       |
| (1,1573) | 1:113:A:ILE:HD12 | 1:106:A:ALA:HB1  | 20                  | 1.13     | 0.08                | 1.12       |
| (1,1573) | 1:113:A:ILE:HD11 | 1:106:A:ALA:HB2  | 20                  | 1.13     | 0.08                | 1.12       |
| (1,1573) | 1:113:A:ILE:HD11 | 1:106:A:ALA:HB3  | 20                  | 1.13     | 0.08                | 1.12       |
| (1,1573) | 1:113:A:ILE:HD13 | 1:106:A:ALA:HB2  | 20                  | 1.13     | 0.08                | 1.12       |
| (1,1573) | 1:113:A:ILE:HD12 | 1:106:A:ALA:HB2  | 20                  | 1.13     | 0.08                | 1.12       |
| (1,1573) | 1:113:A:ILE:HD12 | 1:106:A:ALA:HB3  | 20                  | 1.13     | 0.08                | 1.12       |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 20                  | 1.08     | 0.2                 | 1.18       |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB1   | 20                  | 0.99     | 0.61                | 0.58       |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB2   | 20                  | 0.99     | 0.61                | 0.58       |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB3   | 20                  | 0.99     | 0.61                | 0.58       |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG21  | 20                  | 0.98     | 0.61                | 0.79       |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG22  | 20                  | 0.98     | 0.61                | 0.79       |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG23  | 20                  | 0.98     | 0.61                | 0.79       |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 20                  | 0.97     | 0.37                | 0.92       |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 20                  | 0.96     | 0.17                | 0.92       |
| (3,179)  | 1:148:A:GLU:HA   | 1:18:A:LEU:HD22  | 20                  | 0.9      | 0.64                | 0.64       |
| (3,179)  | 1:148:A:GLU:HA   | 1:18:A:LEU:HD23  | 20                  | 0.9      | 0.64                | 0.64       |
| (3,179)  | 1:148:A:GLU:HA   | 1:152:A:LEU:HD23 | 20                  | 0.9      | 0.64                | 0.64       |
| (3,179)  | 1:148:A:GLU:HA   | 1:152:A:LEU:HD22 | 20                  | 0.9      | 0.64                | 0.64       |
| (3,179)  | 1:148:A:GLU:HA   | 1:152:A:LEU:HD21 | 20                  | 0.9      | 0.64                | 0.64       |
| (3,179)  | 1:148:A:GLU:HA   | 1:18:A:LEU:HD21  | 20                  | 0.9      | 0.64                | 0.64       |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB2   | 20                  | 0.89     | 0.12                | 0.92       |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB1   | 20                  | 0.89     | 0.12                | 0.92       |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB3   | 20                  | 0.89     | 0.12                | 0.92       |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 20                  | 0.89     | 0.08                | 0.88       |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 20                  | 0.89     | 0.21                | 0.9        |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 20                  | 0.84     | 0.78                | 0.21       |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 20                  | 0.83     | 0.2                 | 0.85       |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 20                  | 0.82     | 0.2                 | 0.85       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2  | 20                  | 0.71     | 0.18                | 0.7        |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3  | 20                  | 0.68     | 0.07                | 0.71       |
| (1,1543) | 1:156:A:ALA:HB3  | 1:154:A:ASN:HA  | 20                  | 0.62     | 0.14                | 0.64       |
| (1,1543) | 1:156:A:ALA:HB2  | 1:154:A:ASN:HA  | 20                  | 0.62     | 0.14                | 0.64       |
| (1,1543) | 1:156:A:ALA:HB1  | 1:154:A:ASN:HA  | 20                  | 0.62     | 0.14                | 0.64       |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2  | 20                  | 0.62     | 0.2                 | 0.6        |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD12 | 20                  | 0.62     | 0.41                | 0.55       |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD13 | 20                  | 0.62     | 0.41                | 0.55       |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD11 | 20                  | 0.62     | 0.41                | 0.55       |
| (1,1595) | 1:16:A:ALA:HB3   | 1:19:A:PHE:HD1  | 20                  | 0.61     | 0.11                | 0.62       |
| (1,1595) | 1:16:A:ALA:HB2   | 1:19:A:PHE:HD1  | 20                  | 0.61     | 0.11                | 0.62       |
| (1,1595) | 1:16:A:ALA:HB3   | 1:19:A:PHE:HD2  | 20                  | 0.61     | 0.11                | 0.62       |
| (1,1595) | 1:16:A:ALA:HB1   | 1:19:A:PHE:HD1  | 20                  | 0.61     | 0.11                | 0.62       |
| (1,1595) | 1:16:A:ALA:HB2   | 1:19:A:PHE:HD2  | 20                  | 0.61     | 0.11                | 0.62       |
| (1,1595) | 1:16:A:ALA:HB1   | 1:19:A:PHE:HD2  | 20                  | 0.61     | 0.11                | 0.62       |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2  | 20                  | 0.59     | 0.07                | 0.6        |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HG3  | 20                  | 0.59     | 0.07                | 0.6        |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3 | 20                  | 0.58     | 0.16                | 0.62       |
| (1,955)  | 1:11:A:THR:HG23  | 1:9:A:THR:HA    | 20                  | 0.54     | 0.06                | 0.54       |
| (1,955)  | 1:11:A:THR:HG22  | 1:9:A:THR:HA    | 20                  | 0.54     | 0.06                | 0.54       |
| (1,955)  | 1:11:A:THR:HG21  | 1:9:A:THR:HA    | 20                  | 0.54     | 0.06                | 0.54       |
| (1,1018) | 1:16:A:ALA:HB1   | 1:17:A:ARG:HA   | 20                  | 0.52     | 0.02                | 0.52       |
| (1,1018) | 1:16:A:ALA:HB3   | 1:17:A:ARG:HA   | 20                  | 0.52     | 0.02                | 0.52       |
| (1,1018) | 1:16:A:ALA:HB2   | 1:17:A:ARG:HA   | 20                  | 0.52     | 0.02                | 0.52       |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HB2   | 20                  | 0.51     | 0.29                | 0.4        |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2   | 20                  | 0.51     | 0.29                | 0.4        |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB3  | 20                  | 0.51     | 0.08                | 0.53       |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB2  | 20                  | 0.51     | 0.08                | 0.53       |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB1  | 20                  | 0.51     | 0.08                | 0.53       |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3 | 20                  | 0.5      | 0.03                | 0.5        |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG23 | 20                  | 0.49     | 0.07                | 0.48       |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG21 | 20                  | 0.49     | 0.07                | 0.48       |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG22 | 20                  | 0.49     | 0.07                | 0.48       |
| (1,1589) | 1:105:A:VAL:HG11 | 1:107:A:SER:H   | 20                  | 0.46     | 0.71                | 0.3        |
| (1,1589) | 1:105:A:VAL:HG12 | 1:107:A:SER:H   | 20                  | 0.46     | 0.71                | 0.3        |
| (1,1589) | 1:105:A:VAL:HG13 | 1:107:A:SER:H   | 20                  | 0.46     | 0.71                | 0.3        |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA  | 20                  | 0.45     | 0.13                | 0.41       |
| (1,929)  | 1:9:A:THR:HG23   | 1:22:A:PHE:HD2  | 20                  | 0.44     | 0.05                | 0.45       |
| (1,929)  | 1:9:A:THR:HG21   | 1:22:A:PHE:HD1  | 20                  | 0.44     | 0.05                | 0.45       |
| (1,929)  | 1:9:A:THR:HG23   | 1:22:A:PHE:HD1  | 20                  | 0.44     | 0.05                | 0.45       |
| (1,929)  | 1:9:A:THR:HG22   | 1:22:A:PHE:HD2  | 20                  | 0.44     | 0.05                | 0.45       |
| (1,929)  | 1:9:A:THR:HG21   | 1:22:A:PHE:HD2  | 20                  | 0.44     | 0.05                | 0.45       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,929)  | 1:9:A:THR:HG22   | 1:22:A:PHE:HD1  | 20                  | 0.44     | 0.05                | 0.45       |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3 | 20                  | 0.43     | 0.21                | 0.42       |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD12 | 20                  | 0.43     | 0.19                | 0.43       |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD13 | 20                  | 0.43     | 0.19                | 0.43       |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD11 | 20                  | 0.43     | 0.19                | 0.43       |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2 | 20                  | 0.42     | 0.07                | 0.42       |
| (1,1166) | 1:33:A:VAL:HG13  | 1:29:A:LEU:H    | 20                  | 0.41     | 0.12                | 0.45       |
| (1,1166) | 1:33:A:VAL:HG11  | 1:29:A:LEU:H    | 20                  | 0.41     | 0.12                | 0.45       |
| (1,1166) | 1:33:A:VAL:HG12  | 1:29:A:LEU:H    | 20                  | 0.41     | 0.12                | 0.45       |
| (1,1510) | 1:84:A:THR:HG22  | 1:69:A:HIS:HA   | 20                  | 0.39     | 0.04                | 0.39       |
| (1,1510) | 1:84:A:THR:HG23  | 1:69:A:HIS:HA   | 20                  | 0.39     | 0.04                | 0.39       |
| (1,1510) | 1:84:A:THR:HG21  | 1:69:A:HIS:HA   | 20                  | 0.39     | 0.04                | 0.39       |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3  | 20                  | 0.39     | 0.04                | 0.4        |
| (1,1696) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HB  | 20                  | 0.33     | 0.12                | 0.3        |
| (1,1696) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HB  | 20                  | 0.33     | 0.12                | 0.3        |
| (1,1696) | 1:151:A:LEU:HD13 | 1:147:A:VAL:HB  | 20                  | 0.33     | 0.12                | 0.3        |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2 | 20                  | 0.29     | 0.04                | 0.28       |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB1  | 20                  | 0.25     | 0.05                | 0.24       |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB2  | 20                  | 0.25     | 0.05                | 0.24       |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB3  | 20                  | 0.25     | 0.05                | 0.24       |
| (1,1245) | 1:44:A:ILE:HG21  | 1:44:A:ILE:HB   | 20                  | 0.23     | 0.03                | 0.24       |
| (1,1245) | 1:44:A:ILE:HG22  | 1:44:A:ILE:HB   | 20                  | 0.23     | 0.03                | 0.24       |
| (1,1245) | 1:44:A:ILE:HG23  | 1:44:A:ILE:HB   | 20                  | 0.23     | 0.03                | 0.24       |
| (1,940)  | 1:10:A:THR:HG21  | 1:107:A:SER:HB2 | 20                  | 0.22     | 0.18                | 0.17       |
| (1,940)  | 1:10:A:THR:HG23  | 1:107:A:SER:HB2 | 20                  | 0.22     | 0.18                | 0.17       |
| (1,940)  | 1:10:A:THR:HG22  | 1:107:A:SER:HB2 | 20                  | 0.22     | 0.18                | 0.17       |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA   | 20                  | 0.2      | 0.03                | 0.21       |
| (1,1311) | 1:71:A:ILE:HD13  | 1:71:A:ILE:HG12 | 20                  | 0.2      | 0.01                | 0.2        |
| (1,1311) | 1:71:A:ILE:HD12  | 1:71:A:ILE:HG12 | 20                  | 0.2      | 0.01                | 0.2        |
| (1,1311) | 1:71:A:ILE:HD11  | 1:71:A:ILE:HG12 | 20                  | 0.2      | 0.01                | 0.2        |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG21 | 20                  | 0.17     | 0.01                | 0.17       |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG23 | 20                  | 0.17     | 0.01                | 0.17       |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG22 | 20                  | 0.17     | 0.01                | 0.17       |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB2 | 20                  | 0.14     | 0.01                | 0.14       |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB1 | 20                  | 0.14     | 0.01                | 0.14       |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB3 | 20                  | 0.14     | 0.01                | 0.14       |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3  | 20                  | 0.13     | 0.0                 | 0.13       |
| (1,1557) | 1:85:A:LEU:HD11  | 1:91:A:ILE:HG12 | 19                  | 1.09     | 0.96                | 0.72       |
| (1,1557) | 1:85:A:LEU:HD13  | 1:91:A:ILE:HG12 | 19                  | 1.09     | 0.96                | 0.72       |
| (1,1557) | 1:85:A:LEU:HD12  | 1:91:A:ILE:HG12 | 19                  | 1.09     | 0.96                | 0.72       |
| (1,996)  | 1:82:A:ALA:HB1   | 1:73:A:GLU:HG3  | 19                  | 1.04     | 0.23                | 1.11       |
| (1,996)  | 1:82:A:ALA:HB2   | 1:73:A:GLU:HG3  | 19                  | 1.04     | 0.23                | 1.11       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,996)  | 1:82:A:ALA:HB3   | 1:73:A:GLU:HG3   | 19                  | 1.04     | 0.23                | 1.11       |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG13 | 19                  | 0.87     | 0.1                 | 0.88       |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG12 | 19                  | 0.87     | 0.1                 | 0.88       |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG11 | 19                  | 0.87     | 0.1                 | 0.88       |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 19                  | 0.82     | 0.42                | 0.84       |
| (1,885)  | 1:2:A:VAL:HG21   | 1:4:A:THR:HG21   | 19                  | 0.73     | 0.24                | 0.66       |
| (1,885)  | 1:2:A:VAL:HG21   | 1:4:A:THR:HG23   | 19                  | 0.73     | 0.24                | 0.66       |
| (1,885)  | 1:2:A:VAL:HG22   | 1:4:A:THR:HG21   | 19                  | 0.73     | 0.24                | 0.66       |
| (1,885)  | 1:2:A:VAL:HG23   | 1:4:A:THR:HG21   | 19                  | 0.73     | 0.24                | 0.66       |
| (1,885)  | 1:2:A:VAL:HG23   | 1:4:A:THR:HG22   | 19                  | 0.73     | 0.24                | 0.66       |
| (1,885)  | 1:2:A:VAL:HG22   | 1:4:A:THR:HG23   | 19                  | 0.73     | 0.24                | 0.66       |
| (1,885)  | 1:2:A:VAL:HG23   | 1:4:A:THR:HG23   | 19                  | 0.73     | 0.24                | 0.66       |
| (1,885)  | 1:2:A:VAL:HG21   | 1:4:A:THR:HG22   | 19                  | 0.73     | 0.24                | 0.66       |
| (1,885)  | 1:2:A:VAL:HG22   | 1:4:A:THR:HG22   | 19                  | 0.73     | 0.24                | 0.66       |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 19                  | 0.53     | 0.13                | 0.49       |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB3  | 19                  | 0.48     | 0.07                | 0.49       |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB1  | 19                  | 0.48     | 0.07                | 0.49       |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB2  | 19                  | 0.48     | 0.07                | 0.49       |
| (1,1588) | 1:105:A:VAL:HG11 | 1:105:A:VAL:H    | 19                  | 0.42     | 0.03                | 0.42       |
| (1,1588) | 1:105:A:VAL:HG12 | 1:105:A:VAL:H    | 19                  | 0.42     | 0.03                | 0.42       |
| (1,1588) | 1:105:A:VAL:HG13 | 1:105:A:VAL:H    | 19                  | 0.42     | 0.03                | 0.42       |
| (1,1574) | 1:128:A:ILE:HD12 | 1:91:A:ILE:HD12  | 19                  | 0.28     | 0.15                | 0.2        |
| (1,1574) | 1:128:A:ILE:HD13 | 1:91:A:ILE:HD12  | 19                  | 0.28     | 0.15                | 0.2        |
| (1,1574) | 1:128:A:ILE:HD11 | 1:91:A:ILE:HD12  | 19                  | 0.28     | 0.15                | 0.2        |
| (1,1574) | 1:128:A:ILE:HD13 | 1:91:A:ILE:HD13  | 19                  | 0.28     | 0.15                | 0.2        |
| (1,1574) | 1:128:A:ILE:HD11 | 1:91:A:ILE:HD13  | 19                  | 0.28     | 0.15                | 0.2        |
| (1,1574) | 1:128:A:ILE:HD11 | 1:91:A:ILE:HD11  | 19                  | 0.28     | 0.15                | 0.2        |
| (1,1574) | 1:128:A:ILE:HD12 | 1:91:A:ILE:HD11  | 19                  | 0.28     | 0.15                | 0.2        |
| (1,1461) | 1:74:A:ILE:HG21  | 1:76:A:ASN:H     | 19                  | 0.26     | 0.03                | 0.26       |
| (1,1461) | 1:74:A:ILE:HG22  | 1:76:A:ASN:H     | 19                  | 0.26     | 0.03                | 0.26       |
| (1,1461) | 1:74:A:ILE:HG23  | 1:76:A:ASN:H     | 19                  | 0.26     | 0.03                | 0.26       |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 19                  | 0.26     | 0.07                | 0.26       |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 19                  | 0.21     | 0.07                | 0.17       |
| (3,14)   | 1:24:A:LEU:H     | 1:71:A:ILE:HD13  | 18                  | 1.21     | 0.35                | 1.28       |
| (3,14)   | 1:24:A:LEU:H     | 1:151:A:LEU:HD12 | 18                  | 1.21     | 0.35                | 1.28       |
| (3,14)   | 1:24:A:LEU:H     | 1:71:A:ILE:HD11  | 18                  | 1.21     | 0.35                | 1.28       |
| (3,14)   | 1:24:A:LEU:H     | 1:71:A:ILE:HD12  | 18                  | 1.21     | 0.35                | 1.28       |
| (3,14)   | 1:24:A:LEU:H     | 1:104:A:LEU:HD21 | 18                  | 1.21     | 0.35                | 1.28       |
| (3,14)   | 1:24:A:LEU:H     | 1:104:A:LEU:HD22 | 18                  | 1.21     | 0.35                | 1.28       |
| (3,14)   | 1:24:A:LEU:H     | 1:151:A:LEU:HD13 | 18                  | 1.21     | 0.35                | 1.28       |
| (3,14)   | 1:24:A:LEU:H     | 1:104:A:LEU:HD13 | 18                  | 1.21     | 0.35                | 1.28       |
| (3,14)   | 1:24:A:LEU:H     | 1:104:A:LEU:HD11 | 18                  | 1.21     | 0.35                | 1.28       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD11 | 18                  | 0.92     | 0.59                | 0.72       |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD12 | 18                  | 0.92     | 0.59                | 0.72       |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD13 | 18                  | 0.92     | 0.59                | 0.72       |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 18                  | 0.87     | 0.78                | 0.3        |
| (1,1183) | 1:34:A:ALA:HB3   | 1:147:A:VAL:HG11 | 18                  | 0.78     | 1.0                 | 0.36       |
| (1,1183) | 1:34:A:ALA:HB1   | 1:147:A:VAL:HG11 | 18                  | 0.78     | 1.0                 | 0.36       |
| (1,1183) | 1:34:A:ALA:HB1   | 1:147:A:VAL:HG12 | 18                  | 0.78     | 1.0                 | 0.36       |
| (1,1183) | 1:34:A:ALA:HB1   | 1:147:A:VAL:HG13 | 18                  | 0.78     | 1.0                 | 0.36       |
| (1,1183) | 1:34:A:ALA:HB3   | 1:147:A:VAL:HG12 | 18                  | 0.78     | 1.0                 | 0.36       |
| (1,1183) | 1:34:A:ALA:HB2   | 1:147:A:VAL:HG11 | 18                  | 0.78     | 1.0                 | 0.36       |
| (1,1183) | 1:34:A:ALA:HB2   | 1:147:A:VAL:HG12 | 18                  | 0.78     | 1.0                 | 0.36       |
| (1,1183) | 1:34:A:ALA:HB2   | 1:147:A:VAL:HG13 | 18                  | 0.78     | 1.0                 | 0.36       |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 18                  | 0.68     | 0.33                | 0.78       |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD23  | 18                  | 0.65     | 0.23                | 0.72       |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD21  | 18                  | 0.65     | 0.23                | 0.72       |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD22  | 18                  | 0.65     | 0.23                | 0.72       |
| (1,1204) | 1:38:A:ILE:HD13  | 1:58:A:PHE:HZ    | 18                  | 0.53     | 0.14                | 0.51       |
| (1,1204) | 1:38:A:ILE:HD11  | 1:58:A:PHE:HZ    | 18                  | 0.53     | 0.14                | 0.51       |
| (1,1204) | 1:38:A:ILE:HD12  | 1:58:A:PHE:HZ    | 18                  | 0.53     | 0.14                | 0.51       |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 18                  | 0.37     | 0.17                | 0.38       |
| (1,995)  | 1:82:A:ALA:HB2   | 1:81:A:TYR:HB2   | 18                  | 0.28     | 0.06                | 0.28       |
| (1,995)  | 1:82:A:ALA:HB3   | 1:81:A:TYR:HB2   | 18                  | 0.28     | 0.06                | 0.28       |
| (1,995)  | 1:82:A:ALA:HB1   | 1:81:A:TYR:HB2   | 18                  | 0.28     | 0.06                | 0.28       |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 18                  | 0.28     | 0.04                | 0.28       |
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD2   | 18                  | 0.2      | 0.08                | 0.18       |
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD1   | 18                  | 0.2      | 0.08                | 0.18       |
| (1,657)  | 1:115:A:LYS:H    | 1:115:A:LYS:HB3  | 18                  | 0.19     | 0.02                | 0.19       |
| (1,771)  | 1:139:A:GLU:H    | 1:136:A:GLY:H    | 18                  | 0.15     | 0.03                | 0.15       |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 17                  | 1.94     | 0.91                | 2.07       |
| (1,1310) | 1:44:A:ILE:HD12  | 1:68:A:LYS:HD2   | 17                  | 1.56     | 0.65                | 1.88       |
| (1,1310) | 1:44:A:ILE:HD13  | 1:68:A:LYS:HD2   | 17                  | 1.56     | 0.65                | 1.88       |
| (1,1310) | 1:44:A:ILE:HD11  | 1:68:A:LYS:HD2   | 17                  | 1.56     | 0.65                | 1.88       |
| (3,141)  | 1:67:A:VAL:HG22  | 1:89:A:ASP:HB2   | 17                  | 1.08     | 0.16                | 1.06       |
| (3,141)  | 1:67:A:VAL:HG22  | 1:89:A:ASP:HB3   | 17                  | 1.08     | 0.16                | 1.06       |
| (3,141)  | 1:67:A:VAL:HG23  | 1:89:A:ASP:HB2   | 17                  | 1.08     | 0.16                | 1.06       |
| (3,141)  | 1:67:A:VAL:HG21  | 1:89:A:ASP:HB3   | 17                  | 1.08     | 0.16                | 1.06       |
| (3,141)  | 1:67:A:VAL:HG21  | 1:89:A:ASP:HB2   | 17                  | 1.08     | 0.16                | 1.06       |
| (3,141)  | 1:67:A:VAL:HG23  | 1:89:A:ASP:HB3   | 17                  | 1.08     | 0.16                | 1.06       |
| (1,1618) | 1:114:A:LEU:HD22 | 1:9:A:THR:HB     | 17                  | 1.06     | 0.29                | 1.14       |
| (1,1618) | 1:114:A:LEU:HD21 | 1:9:A:THR:HB     | 17                  | 1.06     | 0.29                | 1.14       |
| (1,1618) | 1:114:A:LEU:HD23 | 1:9:A:THR:HB     | 17                  | 1.06     | 0.29                | 1.14       |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 17                  | 0.46     | 0.25                | 0.41       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE2   | 17                  | 0.41     | 0.14                | 0.38       |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE1   | 17                  | 0.41     | 0.14                | 0.38       |
| (3,37)   | 1:82:A:ALA:H     | 1:70:A:ARG:HE    | 17                  | 0.41     | 0.14                | 0.38       |
| (1,1694) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HA   | 17                  | 0.38     | 0.13                | 0.38       |
| (1,1694) | 1:151:A:LEU:HD13 | 1:147:A:VAL:HA   | 17                  | 0.38     | 0.13                | 0.38       |
| (1,1694) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HA   | 17                  | 0.38     | 0.13                | 0.38       |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG21 | 17                  | 0.33     | 0.01                | 0.33       |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG22 | 17                  | 0.33     | 0.01                | 0.33       |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG23 | 17                  | 0.33     | 0.01                | 0.33       |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 17                  | 0.33     | 0.17                | 0.27       |
| (1,1134) | 1:30:A:ILE:HG23  | 1:37:A:ALA:HB1   | 17                  | 0.32     | 0.07                | 0.34       |
| (1,1134) | 1:30:A:ILE:HG21  | 1:37:A:ALA:HB3   | 17                  | 0.32     | 0.07                | 0.34       |
| (1,1134) | 1:30:A:ILE:HG23  | 1:37:A:ALA:HB3   | 17                  | 0.32     | 0.07                | 0.34       |
| (1,1134) | 1:30:A:ILE:HG22  | 1:37:A:ALA:HB1   | 17                  | 0.32     | 0.07                | 0.34       |
| (1,1134) | 1:30:A:ILE:HG21  | 1:37:A:ALA:HB2   | 17                  | 0.32     | 0.07                | 0.34       |
| (1,1134) | 1:30:A:ILE:HG23  | 1:37:A:ALA:HB2   | 17                  | 0.32     | 0.07                | 0.34       |
| (1,1134) | 1:30:A:ILE:HG21  | 1:37:A:ALA:HB1   | 17                  | 0.32     | 0.07                | 0.34       |
| (1,1134) | 1:30:A:ILE:HG22  | 1:37:A:ALA:HB3   | 17                  | 0.32     | 0.07                | 0.34       |
| (1,1134) | 1:30:A:ILE:HG22  | 1:37:A:ALA:HB2   | 17                  | 0.32     | 0.07                | 0.34       |
| (1,540)  | 1:101:A:GLU:H    | 1:116:A:SER:HA   | 17                  | 0.15     | 0.02                | 0.15       |
| (1,793)  | 1:146:A:ALA:H    | 1:143:A:ILE:HB   | 17                  | 0.13     | 0.02                | 0.12       |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 16                  | 0.72     | 0.24                | 0.74       |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 16                  | 0.63     | 0.27                | 0.64       |
| (1,1141) | 1:102:A:ILE:HG22 | 1:116:A:SER:HB3  | 16                  | 0.62     | 0.5                 | 0.34       |
| (1,1141) | 1:102:A:ILE:HG21 | 1:116:A:SER:HB3  | 16                  | 0.62     | 0.5                 | 0.34       |
| (1,1141) | 1:102:A:ILE:HG23 | 1:116:A:SER:HB3  | 16                  | 0.62     | 0.5                 | 0.34       |
| (1,375)  | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 16                  | 0.5      | 0.34                | 0.5        |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3  | 16                  | 0.39     | 0.14                | 0.38       |
| (1,1120) | 1:74:A:ILE:HD11  | 1:71:A:ILE:HA    | 16                  | 0.38     | 0.13                | 0.44       |
| (1,1120) | 1:74:A:ILE:HD12  | 1:71:A:ILE:HA    | 16                  | 0.38     | 0.13                | 0.44       |
| (1,1120) | 1:74:A:ILE:HD13  | 1:71:A:ILE:HA    | 16                  | 0.38     | 0.13                | 0.44       |
| (3,172)  | 1:101:A:GLU:HA   | 1:81:A:TYR:H     | 16                  | 0.22     | 0.06                | 0.22       |
| (3,172)  | 1:101:A:GLU:HA   | 1:100:A:TYR:H    | 16                  | 0.22     | 0.06                | 0.22       |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 15                  | 0.67     | 0.32                | 0.69       |
| (1,1133) | 1:91:A:ILE:HG23  | 1:95:A:LEU:HB3   | 15                  | 0.66     | 0.38                | 0.54       |
| (1,1133) | 1:91:A:ILE:HG21  | 1:95:A:LEU:HB3   | 15                  | 0.66     | 0.38                | 0.54       |
| (1,1133) | 1:91:A:ILE:HG22  | 1:95:A:LEU:HB3   | 15                  | 0.66     | 0.38                | 0.54       |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 15                  | 0.49     | 0.33                | 0.35       |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD12  | 15                  | 0.47     | 0.12                | 0.48       |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD11  | 15                  | 0.47     | 0.12                | 0.48       |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD13  | 15                  | 0.47     | 0.12                | 0.48       |
| (1,976)  | 1:13:A:ILE:HG21  | 1:17:A:ARG:HB2   | 15                  | 0.3      | 0.09                | 0.31       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,976)  | 1:13:A:ILE:HG23  | 1:17:A:ARG:HB2   | 15                  | 0.3      | 0.09                | 0.31       |
| (1,976)  | 1:13:A:ILE:HG22  | 1:17:A:ARG:HB2   | 15                  | 0.3      | 0.09                | 0.31       |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2   | 15                  | 0.23     | 0.1                 | 0.21       |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB3   | 15                  | 0.23     | 0.1                 | 0.21       |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 15                  | 0.16     | 0.03                | 0.16       |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 14                  | 1.52     | 0.48                | 1.38       |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG23 | 14                  | 1.19     | 0.94                | 0.8        |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG21 | 14                  | 1.19     | 0.94                | 0.8        |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG22 | 14                  | 1.19     | 0.94                | 0.8        |
| (1,849)  | 1:17:A:ARG:HH11  | 1:155:A:PRO:HG3  | 14                  | 1.12     | 0.79                | 0.68       |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG21  | 14                  | 0.89     | 0.29                | 1.02       |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG23  | 14                  | 0.89     | 0.29                | 1.02       |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG22  | 14                  | 0.89     | 0.29                | 1.02       |
| (3,23)   | 1:45:A:GLU:H     | 1:43:A:ILE:HD13  | 14                  | 0.89     | 0.29                | 1.02       |
| (1,1450) | 1:71:A:ILE:HG23  | 1:70:A:ARG:HE    | 14                  | 0.51     | 0.15                | 0.56       |
| (1,1450) | 1:71:A:ILE:HG22  | 1:70:A:ARG:HE    | 14                  | 0.51     | 0.15                | 0.56       |
| (1,1450) | 1:71:A:ILE:HG21  | 1:70:A:ARG:HE    | 14                  | 0.51     | 0.15                | 0.56       |
| (1,1127) | 1:71:A:ILE:HG23  | 1:82:A:ALA:HA    | 14                  | 0.49     | 0.16                | 0.53       |
| (1,1127) | 1:71:A:ILE:HG21  | 1:82:A:ALA:HA    | 14                  | 0.49     | 0.16                | 0.53       |
| (1,1127) | 1:71:A:ILE:HG22  | 1:82:A:ALA:HA    | 14                  | 0.49     | 0.16                | 0.53       |
| (1,1203) | 1:38:A:ILE:HD11  | 1:38:A:ILE:HA    | 14                  | 0.39     | 0.04                | 0.38       |
| (1,1203) | 1:38:A:ILE:HD12  | 1:38:A:ILE:HA    | 14                  | 0.39     | 0.04                | 0.38       |
| (1,1203) | 1:38:A:ILE:HD13  | 1:38:A:ILE:HA    | 14                  | 0.39     | 0.04                | 0.38       |
| (3,83)   | 1:55:A:LYS:HE2   | 1:55:A:LYS:HD2   | 14                  | 0.37     | 0.0                 | 0.37       |
| (3,83)   | 1:20:A:LYS:HD2   | 1:20:A:LYS:HE2   | 14                  | 0.37     | 0.0                 | 0.37       |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 14                  | 0.37     | 0.23                | 0.28       |
| (1,479)  | 1:87:A:GLU:H     | 1:68:A:LYS:HB3   | 14                  | 0.35     | 0.11                | 0.37       |
| (1,994)  | 1:82:A:ALA:HB1   | 1:71:A:ILE:HA    | 14                  | 0.28     | 0.09                | 0.28       |
| (1,994)  | 1:82:A:ALA:HB2   | 1:71:A:ILE:HA    | 14                  | 0.28     | 0.09                | 0.28       |
| (1,994)  | 1:82:A:ALA:HB3   | 1:71:A:ILE:HA    | 14                  | 0.28     | 0.09                | 0.28       |
| (1,640)  | 1:113:A:ILE:H    | 1:114:A:LEU:HG   | 14                  | 0.13     | 0.02                | 0.12       |
| (1,957)  | 1:11:A:THR:HG22  | 1:112:A:SER:HB2  | 13                  | 1.5      | 0.87                | 1.97       |
| (1,957)  | 1:11:A:THR:HG21  | 1:112:A:SER:HB2  | 13                  | 1.5      | 0.87                | 1.97       |
| (1,957)  | 1:11:A:THR:HG23  | 1:112:A:SER:HB2  | 13                  | 1.5      | 0.87                | 1.97       |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD23 | 13                  | 1.47     | 1.1                 | 0.92       |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD21 | 13                  | 1.47     | 1.1                 | 0.92       |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD22 | 13                  | 1.47     | 1.1                 | 0.92       |
| (1,70)   | 1:10:A:THR:H     | 1:8:A:GLU:HG3    | 13                  | 1.41     | 0.07                | 1.44       |
| (1,890)  | 1:2:A:VAL:HG13   | 1:4:A:THR:HB     | 13                  | 0.58     | 0.61                | 0.44       |
| (1,890)  | 1:2:A:VAL:HG12   | 1:4:A:THR:HB     | 13                  | 0.58     | 0.61                | 0.44       |
| (1,890)  | 1:2:A:VAL:HG11   | 1:4:A:THR:HB     | 13                  | 0.58     | 0.61                | 0.44       |
| (1,1429) | 1:104:A:LEU:HD12 | 1:106:A:ALA:H    | 13                  | 0.48     | 0.24                | 0.46       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1429) | 1:104:A:LEU:HD11 | 1:106:A:ALA:H    | 13                  | 0.48     | 0.24                | 0.46       |
| (1,1429) | 1:104:A:LEU:HD13 | 1:106:A:ALA:H    | 13                  | 0.48     | 0.24                | 0.46       |
| (1,233)  | 1:70:A:ARG:HH22  | 1:70:A:ARG:HB2   | 13                  | 0.41     | 0.22                | 0.34       |
| (1,96)   | 1:146:A:ALA:H    | 1:145:A:LYS:HB2  | 13                  | 0.38     | 0.06                | 0.38       |
| (1,1514) | 1:18:A:LEU:HD22  | 1:13:A:ILE:HA    | 13                  | 0.38     | 0.13                | 0.35       |
| (1,1514) | 1:18:A:LEU:HD23  | 1:13:A:ILE:HA    | 13                  | 0.38     | 0.13                | 0.35       |
| (1,1514) | 1:18:A:LEU:HD21  | 1:13:A:ILE:HA    | 13                  | 0.38     | 0.13                | 0.35       |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD12  | 13                  | 0.31     | 0.29                | 0.19       |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD13  | 13                  | 0.31     | 0.29                | 0.19       |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD11  | 13                  | 0.31     | 0.29                | 0.19       |
| (1,404)  | 1:75:A:ASP:H     | 1:81:A:TYR:H     | 13                  | 0.13     | 0.02                | 0.13       |
| (1,1159) | 1:103:A:LYS:HG2  | 1:105:A:VAL:HA   | 12                  | 1.3      | 0.22                | 1.4        |
| (1,1529) | 1:123:A:LYS:HA   | 1:96:A:GLU:HG2   | 12                  | 1.3      | 0.11                | 1.31       |
| (1,886)  | 1:2:A:VAL:HG22   | 1:119:A:LYS:HD2  | 12                  | 1.23     | 0.37                | 1.39       |
| (1,886)  | 1:2:A:VAL:HG23   | 1:119:A:LYS:HD2  | 12                  | 1.23     | 0.37                | 1.39       |
| (1,886)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HD2  | 12                  | 1.23     | 0.37                | 1.39       |
| (1,581)  | 1:105:A:VAL:H    | 1:103:A:LYS:HG2  | 12                  | 1.14     | 0.26                | 1.25       |
| (1,884)  | 1:2:A:VAL:HG22   | 1:119:A:LYS:HG3  | 12                  | 0.89     | 0.25                | 0.88       |
| (1,884)  | 1:2:A:VAL:HG23   | 1:119:A:LYS:HG3  | 12                  | 0.89     | 0.25                | 0.88       |
| (1,884)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HG3  | 12                  | 0.89     | 0.25                | 0.88       |
| (1,1524) | 1:20:A:LYS:HB3   | 1:19:A:PHE:HB2   | 12                  | 0.82     | 0.06                | 0.83       |
| (1,565)  | 1:104:A:LEU:H    | 1:103:A:LYS:HG2  | 12                  | 0.57     | 0.08                | 0.56       |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG11 | 12                  | 0.48     | 0.28                | 0.45       |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG12 | 12                  | 0.48     | 0.28                | 0.45       |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG13 | 12                  | 0.48     | 0.28                | 0.45       |
| (1,1271) | 1:48:A:GLY:HA2   | 1:71:A:ILE:HG12  | 12                  | 0.43     | 0.23                | 0.36       |
| (3,151)  | 1:104:A:LEU:HD21 | 1:18:A:LEU:HB3   | 12                  | 0.33     | 0.1                 | 0.29       |
| (3,151)  | 1:104:A:LEU:HD23 | 1:114:A:LEU:HG   | 12                  | 0.33     | 0.1                 | 0.29       |
| (3,151)  | 1:104:A:LEU:HD21 | 1:114:A:LEU:HG   | 12                  | 0.33     | 0.1                 | 0.29       |
| (3,151)  | 1:104:A:LEU:HD22 | 1:18:A:LEU:HB3   | 12                  | 0.33     | 0.1                 | 0.29       |
| (3,151)  | 1:104:A:LEU:HD22 | 1:114:A:LEU:HG   | 12                  | 0.33     | 0.1                 | 0.29       |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG23  | 12                  | 0.27     | 0.01                | 0.28       |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG22  | 12                  | 0.27     | 0.01                | 0.28       |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG21  | 12                  | 0.27     | 0.01                | 0.28       |
| (1,1300) | 1:71:A:ILE:HD11  | 1:70:A:ARG:HE    | 12                  | 0.26     | 0.14                | 0.19       |
| (1,1300) | 1:71:A:ILE:HD12  | 1:70:A:ARG:HE    | 12                  | 0.26     | 0.14                | 0.19       |
| (1,1300) | 1:71:A:ILE:HD13  | 1:70:A:ARG:HE    | 12                  | 0.26     | 0.14                | 0.19       |
| (1,71)   | 1:30:A:ILE:H     | 1:30:A:ILE:HG12  | 12                  | 0.24     | 0.03                | 0.24       |
| (1,1072) | 1:23:A:VAL:HG13  | 1:23:A:VAL:H     | 12                  | 0.15     | 0.03                | 0.15       |
| (1,1072) | 1:23:A:VAL:HG12  | 1:23:A:VAL:H     | 12                  | 0.15     | 0.03                | 0.15       |
| (1,1072) | 1:23:A:VAL:HG11  | 1:23:A:VAL:H     | 12                  | 0.15     | 0.03                | 0.15       |
| (4,33)   | 1:87:A:GLU:H     | 1:68:A:LYS:O     | 12                  | 0.14     | 0.02                | 0.14       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,904)  | 1:4:A:THR:HG21   | 1:6:A:GLU:HG3    | 11                  | 1.55     | 0.5                 | 1.83       |
| (1,904)  | 1:4:A:THR:HG22   | 1:6:A:GLU:HG3    | 11                  | 1.55     | 0.5                 | 1.83       |
| (1,904)  | 1:4:A:THR:HG23   | 1:6:A:GLU:HG3    | 11                  | 1.55     | 0.5                 | 1.83       |
| (1,943)  | 1:117:A:THR:HG23 | 1:101:A:GLU:HB3  | 11                  | 0.93     | 0.59                | 1.17       |
| (1,943)  | 1:117:A:THR:HG21 | 1:101:A:GLU:HB3  | 11                  | 0.93     | 0.59                | 1.17       |
| (1,943)  | 1:117:A:THR:HG22 | 1:101:A:GLU:HB3  | 11                  | 0.93     | 0.59                | 1.17       |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG22 | 11                  | 0.83     | 0.2                 | 0.76       |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG23 | 11                  | 0.83     | 0.2                 | 0.76       |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG21 | 11                  | 0.83     | 0.2                 | 0.76       |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG21  | 11                  | 0.82     | 0.09                | 0.79       |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG22  | 11                  | 0.82     | 0.09                | 0.79       |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG23  | 11                  | 0.82     | 0.09                | 0.79       |
| (1,1111) | 1:30:A:ILE:HA    | 1:147:A:VAL:HG11 | 11                  | 0.63     | 0.69                | 0.27       |
| (1,1111) | 1:30:A:ILE:HA    | 1:147:A:VAL:HG12 | 11                  | 0.63     | 0.69                | 0.27       |
| (1,1111) | 1:30:A:ILE:HA    | 1:147:A:VAL:HG13 | 11                  | 0.63     | 0.69                | 0.27       |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD11  | 11                  | 0.52     | 0.21                | 0.5        |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD12  | 11                  | 0.52     | 0.21                | 0.5        |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD13  | 11                  | 0.52     | 0.21                | 0.5        |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD12  | 11                  | 0.51     | 0.15                | 0.53       |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD13  | 11                  | 0.51     | 0.15                | 0.53       |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD11  | 11                  | 0.51     | 0.15                | 0.53       |
| (1,1697) | 1:151:A:LEU:HD11 | 1:150:A:TYR:HD1  | 11                  | 0.48     | 0.15                | 0.57       |
| (1,1697) | 1:151:A:LEU:HD12 | 1:150:A:TYR:HD1  | 11                  | 0.48     | 0.15                | 0.57       |
| (1,1697) | 1:151:A:LEU:HD11 | 1:150:A:TYR:HD2  | 11                  | 0.48     | 0.15                | 0.57       |
| (1,1697) | 1:151:A:LEU:HD13 | 1:150:A:TYR:HD2  | 11                  | 0.48     | 0.15                | 0.57       |
| (1,1697) | 1:151:A:LEU:HD12 | 1:150:A:TYR:HD2  | 11                  | 0.48     | 0.15                | 0.57       |
| (1,1697) | 1:151:A:LEU:HD13 | 1:150:A:TYR:HD1  | 11                  | 0.48     | 0.15                | 0.57       |
| (1,777)  | 1:142:A:GLY:H    | 1:141:A:SER:HB3  | 11                  | 0.47     | 0.06                | 0.47       |
| (1,1654) | 1:133:A:ILE:HG22 | 1:5:A:TYR:HB2    | 11                  | 0.41     | 0.21                | 0.39       |
| (1,1654) | 1:133:A:ILE:HG23 | 1:5:A:TYR:HB2    | 11                  | 0.41     | 0.21                | 0.39       |
| (1,1654) | 1:133:A:ILE:HG21 | 1:5:A:TYR:HB2    | 11                  | 0.41     | 0.21                | 0.39       |
| (1,1238) | 1:43:A:ILE:HD12  | 1:48:A:GLY:HA2   | 11                  | 0.4      | 0.12                | 0.39       |
| (1,1238) | 1:43:A:ILE:HD13  | 1:48:A:GLY:HA2   | 11                  | 0.4      | 0.12                | 0.39       |
| (1,1238) | 1:43:A:ILE:HD11  | 1:48:A:GLY:HA2   | 11                  | 0.4      | 0.12                | 0.39       |
| (1,1029) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD12 | 11                  | 0.39     | 0.48                | 0.17       |
| (1,1029) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD13 | 11                  | 0.39     | 0.48                | 0.17       |
| (1,1029) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD11 | 11                  | 0.39     | 0.48                | 0.17       |
| (3,167)  | 1:146:A:ALA:HB2  | 1:35:A:PRO:HD3   | 11                  | 0.37     | 0.22                | 0.31       |
| (3,167)  | 1:146:A:ALA:HB3  | 1:35:A:PRO:HD2   | 11                  | 0.37     | 0.22                | 0.31       |
| (3,167)  | 1:146:A:ALA:HB1  | 1:35:A:PRO:HD3   | 11                  | 0.37     | 0.22                | 0.31       |
| (3,167)  | 1:146:A:ALA:HB1  | 1:35:A:PRO:HD2   | 11                  | 0.37     | 0.22                | 0.31       |
| (3,167)  | 1:146:A:ALA:HB2  | 1:35:A:PRO:HD2   | 11                  | 0.37     | 0.22                | 0.31       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG22  | 11                  | 0.34     | 0.08                | 0.3        |
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG23  | 11                  | 0.34     | 0.08                | 0.3        |
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG21  | 11                  | 0.34     | 0.08                | 0.3        |
| (1,625)  | 1:111:A:GLY:H    | 1:109:A:ASP:HA   | 11                  | 0.3      | 0.03                | 0.31       |
| (1,772)  | 1:141:A:SER:H    | 1:141:A:SER:HB3  | 11                  | 0.17     | 0.01                | 0.17       |
| (1,47)   | 1:6:A:GLU:H      | 1:7:A:SER:HA     | 11                  | 0.14     | 0.04                | 0.13       |
| (1,1109) | 1:30:A:ILE:HA    | 1:30:A:ILE:HG12  | 11                  | 0.13     | 0.01                | 0.13       |
| (3,158)  | 1:118:A:SER:HB2  | 1:6:A:GLU:HB2    | 10                  | 0.87     | 0.4                 | 1.03       |
| (3,158)  | 1:118:A:SER:HB2  | 1:6:A:GLU:HG2    | 10                  | 0.87     | 0.4                 | 1.03       |
| (1,1555) | 1:104:A:LEU:HD11 | 1:114:A:LEU:HA   | 10                  | 0.73     | 0.1                 | 0.7        |
| (1,1555) | 1:104:A:LEU:HD13 | 1:114:A:LEU:HA   | 10                  | 0.73     | 0.1                 | 0.7        |
| (1,1555) | 1:104:A:LEU:HD12 | 1:114:A:LEU:HA   | 10                  | 0.73     | 0.1                 | 0.7        |
| (1,1556) | 1:104:A:LEU:HD13 | 1:79:A:PHE:HB3   | 10                  | 0.51     | 0.2                 | 0.54       |
| (1,1556) | 1:104:A:LEU:HD11 | 1:79:A:PHE:HB3   | 10                  | 0.51     | 0.2                 | 0.54       |
| (1,1556) | 1:104:A:LEU:HD12 | 1:79:A:PHE:HB3   | 10                  | 0.51     | 0.2                 | 0.54       |
| (1,1579) | 1:104:A:LEU:HA   | 1:104:A:LEU:HG   | 10                  | 0.31     | 0.07                | 0.33       |
| (1,1168) | 1:33:A:VAL:HG12  | 1:150:A:TYR:HB3  | 10                  | 0.3      | 0.14                | 0.26       |
| (1,1168) | 1:33:A:VAL:HG13  | 1:150:A:TYR:HB3  | 10                  | 0.3      | 0.14                | 0.26       |
| (1,1168) | 1:33:A:VAL:HG11  | 1:150:A:TYR:HB3  | 10                  | 0.3      | 0.14                | 0.26       |
| (1,648)  | 1:114:A:LEU:H    | 1:113:A:ILE:HG23 | 10                  | 0.13     | 0.02                | 0.12       |
| (1,648)  | 1:114:A:LEU:H    | 1:113:A:ILE:HG21 | 10                  | 0.13     | 0.02                | 0.12       |
| (1,648)  | 1:114:A:LEU:H    | 1:113:A:ILE:HG22 | 10                  | 0.13     | 0.02                | 0.12       |
| (1,1012) | 1:138:A:GLU:HB3  | 1:136:A:GLY:H    | 9                   | 1.73     | 0.02                | 1.74       |
| (1,1154) | 1:96:A:GLU:HA    | 1:123:A:LYS:HD3  | 9                   | 1.21     | 0.33                | 1.27       |
| (1,1612) | 1:112:A:SER:HB2  | 1:11:A:THR:HA    | 9                   | 1.17     | 0.11                | 1.23       |
| (1,1030) | 1:55:A:LYS:HE3   | 1:44:A:ILE:HD13  | 9                   | 1.06     | 0.39                | 1.13       |
| (1,1030) | 1:55:A:LYS:HE3   | 1:44:A:ILE:HD12  | 9                   | 1.06     | 0.39                | 1.13       |
| (1,1030) | 1:55:A:LYS:HE3   | 1:44:A:ILE:HD11  | 9                   | 1.06     | 0.39                | 1.13       |
| (1,1350) | 1:56:A:ILE:HG23  | 1:38:A:ILE:HG12  | 9                   | 1.03     | 0.55                | 1.22       |
| (1,1350) | 1:56:A:ILE:HG21  | 1:38:A:ILE:HG12  | 9                   | 1.03     | 0.55                | 1.22       |
| (1,1350) | 1:56:A:ILE:HG22  | 1:38:A:ILE:HG12  | 9                   | 1.03     | 0.55                | 1.22       |
| (1,604)  | 1:107:A:SER:H    | 1:110:A:GLY:HA2  | 9                   | 1.0      | 0.08                | 1.0        |
| (1,765)  | 1:139:A:GLU:H    | 1:138:A:GLU:HB3  | 9                   | 0.78     | 0.05                | 0.77       |
| (3,58)   | 1:121:A:HIS:H    | 1:91:A:ILE:HD12  | 9                   | 0.5      | 0.17                | 0.45       |
| (3,58)   | 1:121:A:HIS:H    | 1:128:A:ILE:HG12 | 9                   | 0.5      | 0.17                | 0.45       |
| (3,58)   | 1:121:A:HIS:H    | 1:91:A:ILE:HD11  | 9                   | 0.5      | 0.17                | 0.45       |
| (1,1678) | 1:134:A:LYS:HA   | 1:134:A:LYS:HD3  | 9                   | 0.49     | 0.33                | 0.3        |
| (1,344)  | 1:64:A:PHE:H     | 1:57:A:THR:HG21  | 9                   | 0.41     | 0.28                | 0.27       |
| (1,344)  | 1:64:A:PHE:H     | 1:57:A:THR:HG22  | 9                   | 0.41     | 0.28                | 0.27       |
| (1,344)  | 1:64:A:PHE:H     | 1:57:A:THR:HG23  | 9                   | 0.41     | 0.28                | 0.27       |
| (1,95)   | 1:13:A:ILE:H     | 1:12:A:VAL:HG12  | 9                   | 0.41     | 0.53                | 0.24       |
| (1,95)   | 1:13:A:ILE:H     | 1:12:A:VAL:HG11  | 9                   | 0.41     | 0.53                | 0.24       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,95)   | 1:13:A:ILE:H     | 1:12:A:VAL:HG13  | 9                   | 0.41     | 0.53                | 0.24       |
| (1,1551) | 1:114:A:LEU:HA   | 1:104:A:LEU:HD23 | 9                   | 0.35     | 0.45                | 0.21       |
| (1,1551) | 1:114:A:LEU:HA   | 1:104:A:LEU:HD22 | 9                   | 0.35     | 0.45                | 0.21       |
| (1,1551) | 1:114:A:LEU:HA   | 1:104:A:LEU:HD21 | 9                   | 0.35     | 0.45                | 0.21       |
| (1,1661) | 1:143:A:ILE:HA   | 1:37:A:ALA:HB3   | 9                   | 0.28     | 0.14                | 0.25       |
| (1,1661) | 1:143:A:ILE:HA   | 1:37:A:ALA:HB1   | 9                   | 0.28     | 0.14                | 0.25       |
| (1,1661) | 1:143:A:ILE:HA   | 1:37:A:ALA:HB2   | 9                   | 0.28     | 0.14                | 0.25       |
| (1,1289) | 1:52:A:THR:HB    | 1:71:A:ILE:HG22  | 9                   | 0.27     | 0.12                | 0.27       |
| (1,1289) | 1:52:A:THR:HB    | 1:71:A:ILE:HG23  | 9                   | 0.27     | 0.12                | 0.27       |
| (1,1289) | 1:52:A:THR:HB    | 1:71:A:ILE:HG21  | 9                   | 0.27     | 0.12                | 0.27       |
| (1,839)  | 1:154:A:ASN:H    | 1:153:A:ALA:HB3  | 9                   | 0.19     | 0.05                | 0.2        |
| (1,839)  | 1:154:A:ASN:H    | 1:153:A:ALA:HB2  | 9                   | 0.19     | 0.05                | 0.2        |
| (1,839)  | 1:154:A:ASN:H    | 1:153:A:ALA:HB1  | 9                   | 0.19     | 0.05                | 0.2        |
| (1,822)  | 1:153:A:ALA:H    | 1:151:A:LEU:H    | 9                   | 0.13     | 0.01                | 0.13       |
| (1,1054) | 1:22:A:PHE:HA    | 1:29:A:LEU:HD13  | 8                   | 1.28     | 0.98                | 1.45       |
| (1,1054) | 1:22:A:PHE:HA    | 1:29:A:LEU:HD12  | 8                   | 1.28     | 0.98                | 1.45       |
| (1,1536) | 1:68:A:LYS:HE2   | 1:44:A:ILE:HD12  | 8                   | 0.94     | 0.09                | 0.94       |
| (1,1536) | 1:68:A:LYS:HE2   | 1:44:A:ILE:HD11  | 8                   | 0.94     | 0.09                | 0.94       |
| (1,477)  | 1:87:A:GLU:H     | 1:67:A:VAL:HG23  | 8                   | 0.86     | 1.1                 | 0.31       |
| (1,477)  | 1:87:A:GLU:H     | 1:67:A:VAL:HG22  | 8                   | 0.86     | 1.1                 | 0.31       |
| (1,477)  | 1:87:A:GLU:H     | 1:67:A:VAL:HG21  | 8                   | 0.86     | 1.1                 | 0.31       |
| (1,1233) | 1:133:A:ILE:HG13 | 1:128:A:ILE:HB   | 8                   | 0.75     | 0.31                | 0.86       |
| (1,1624) | 1:118:A:SER:HB2  | 1:119:A:LYS:HB2  | 8                   | 0.65     | 0.27                | 0.8        |
| (1,882)  | 1:2:A:VAL:HG22   | 1:119:A:LYS:HE2  | 8                   | 0.52     | 0.15                | 0.47       |
| (1,882)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HE2  | 8                   | 0.52     | 0.15                | 0.47       |
| (1,882)  | 1:2:A:VAL:HG23   | 1:119:A:LYS:HE2  | 8                   | 0.52     | 0.15                | 0.47       |
| (1,823)  | 1:153:A:ALA:H    | 1:17:A:ARG:HH11  | 8                   | 0.35     | 0.15                | 0.46       |
| (1,1340) | 1:128:A:ILE:HD13 | 1:98:A:ILE:HG23  | 8                   | 0.35     | 0.22                | 0.29       |
| (1,1340) | 1:128:A:ILE:HD11 | 1:98:A:ILE:HG23  | 8                   | 0.35     | 0.22                | 0.29       |
| (1,1340) | 1:128:A:ILE:HD12 | 1:98:A:ILE:HG22  | 8                   | 0.35     | 0.22                | 0.29       |
| (1,1340) | 1:128:A:ILE:HD13 | 1:98:A:ILE:HG21  | 8                   | 0.35     | 0.22                | 0.29       |
| (1,1340) | 1:128:A:ILE:HD11 | 1:98:A:ILE:HG21  | 8                   | 0.35     | 0.22                | 0.29       |
| (1,1660) | 1:143:A:ILE:HA   | 1:144:A:PHE:HD2  | 8                   | 0.32     | 0.16                | 0.26       |
| (1,1660) | 1:143:A:ILE:HA   | 1:144:A:PHE:HD1  | 8                   | 0.32     | 0.16                | 0.26       |
| (1,859)  | 1:78:A:ASN:HD21  | 1:77:A:ALA:HB3   | 8                   | 0.24     | 0.12                | 0.21       |
| (1,859)  | 1:78:A:ASN:HD21  | 1:77:A:ALA:HB1   | 8                   | 0.24     | 0.12                | 0.21       |
| (1,859)  | 1:78:A:ASN:HD21  | 1:77:A:ALA:HB2   | 8                   | 0.24     | 0.12                | 0.21       |
| (1,939)  | 1:80:A:THR:HG23  | 1:74:A:ILE:HA    | 8                   | 0.22     | 0.08                | 0.21       |
| (1,939)  | 1:80:A:THR:HG21  | 1:74:A:ILE:HA    | 8                   | 0.22     | 0.08                | 0.21       |
| (1,939)  | 1:80:A:THR:HG22  | 1:74:A:ILE:HA    | 8                   | 0.22     | 0.08                | 0.21       |
| (1,1351) | 1:56:A:ILE:HG23  | 1:38:A:ILE:HG22  | 8                   | 0.2      | 0.07                | 0.18       |
| (1,1351) | 1:56:A:ILE:HG22  | 1:38:A:ILE:HG21  | 8                   | 0.2      | 0.07                | 0.18       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1351) | 1:56:A:ILE:HG22  | 1:38:A:ILE:HG23  | 8                   | 0.2      | 0.07                | 0.18       |
| (1,1351) | 1:56:A:ILE:HG21  | 1:38:A:ILE:HG23  | 8                   | 0.2      | 0.07                | 0.18       |
| (1,1351) | 1:56:A:ILE:HG23  | 1:38:A:ILE:HG21  | 8                   | 0.2      | 0.07                | 0.18       |
| (1,1351) | 1:56:A:ILE:HG21  | 1:38:A:ILE:HG22  | 8                   | 0.2      | 0.07                | 0.18       |
| (1,1351) | 1:56:A:ILE:HG21  | 1:38:A:ILE:HG21  | 8                   | 0.2      | 0.07                | 0.18       |
| (1,307)  | 1:55:A:LYS:H     | 1:55:A:LYS:HG2   | 8                   | 0.12     | 0.01                | 0.12       |
| (4,34)   | 1:87:A:GLU:N     | 1:68:A:LYS:O     | 8                   | 0.11     | 0.01                | 0.11       |
| (1,1126) | 1:139:A:GLU:HB2  | 1:136:A:GLY:H    | 7                   | 1.53     | 0.05                | 1.54       |
| (1,1531) | 1:19:A:PHE:HB2   | 1:20:A:LYS:HG2   | 7                   | 1.4      | 0.76                | 1.88       |
| (3,154)  | 1:85:A:LEU:HD21  | 1:83:A:CYS:HB3   | 7                   | 1.13     | 0.73                | 0.61       |
| (3,154)  | 1:85:A:LEU:HD21  | 1:97:A:LYS:HE3   | 7                   | 1.13     | 0.73                | 0.61       |
| (3,154)  | 1:85:A:LEU:HD23  | 1:83:A:CYS:HB3   | 7                   | 1.13     | 0.73                | 0.61       |
| (3,154)  | 1:85:A:LEU:HD22  | 1:83:A:CYS:HB3   | 7                   | 1.13     | 0.73                | 0.61       |
| (1,1281) | 1:155:A:PRO:HD3  | 1:151:A:LEU:HD21 | 7                   | 1.03     | 1.42                | 0.22       |
| (1,1281) | 1:155:A:PRO:HD3  | 1:151:A:LEU:HD22 | 7                   | 1.03     | 1.42                | 0.22       |
| (1,1281) | 1:155:A:PRO:HD3  | 1:151:A:LEU:HD23 | 7                   | 1.03     | 1.42                | 0.22       |
| (1,1675) | 1:147:A:VAL:HG23 | 1:22:A:PHE:HB2   | 7                   | 0.94     | 0.6                 | 0.73       |
| (1,1675) | 1:147:A:VAL:HG21 | 1:22:A:PHE:HB2   | 7                   | 0.94     | 0.6                 | 0.73       |
| (1,1682) | 1:149:A:ALA:HA   | 1:152:A:LEU:HD21 | 7                   | 0.75     | 0.36                | 0.61       |
| (1,1682) | 1:149:A:ALA:HA   | 1:152:A:LEU:HD22 | 7                   | 0.75     | 0.36                | 0.61       |
| (1,1682) | 1:149:A:ALA:HA   | 1:152:A:LEU:HD23 | 7                   | 0.75     | 0.36                | 0.61       |
| (1,764)  | 1:139:A:GLU:H    | 1:139:A:GLU:HB2  | 7                   | 0.57     | 0.02                | 0.57       |
| (1,310)  | 1:56:A:ILE:H     | 1:67:A:VAL:HG12  | 7                   | 0.54     | 0.65                | 0.22       |
| (1,310)  | 1:56:A:ILE:H     | 1:67:A:VAL:HG11  | 7                   | 0.54     | 0.65                | 0.22       |
| (1,310)  | 1:56:A:ILE:H     | 1:67:A:VAL:HG13  | 7                   | 0.54     | 0.65                | 0.22       |
| (1,1541) | 1:143:A:ILE:HA   | 1:30:A:ILE:HG12  | 7                   | 0.53     | 0.28                | 0.6        |
| (1,875)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:H    | 7                   | 0.45     | 0.27                | 0.44       |
| (1,1335) | 1:128:A:ILE:HD12 | 1:128:A:ILE:HA   | 7                   | 0.33     | 0.1                 | 0.27       |
| (1,1335) | 1:128:A:ILE:HD11 | 1:128:A:ILE:HA   | 7                   | 0.33     | 0.1                 | 0.27       |
| (1,1335) | 1:128:A:ILE:HD13 | 1:128:A:ILE:HA   | 7                   | 0.33     | 0.1                 | 0.27       |
| (1,449)  | 1:81:A:TYR:H     | 1:19:A:PHE:HD2   | 7                   | 0.12     | 0.02                | 0.12       |
| (1,449)  | 1:81:A:TYR:H     | 1:19:A:PHE:HD1   | 7                   | 0.12     | 0.02                | 0.12       |
| (1,967)  | 1:103:A:LYS:HB2  | 1:80:A:THR:HG23  | 7                   | 0.12     | 0.01                | 0.11       |
| (1,967)  | 1:103:A:LYS:HB2  | 1:80:A:THR:HG21  | 7                   | 0.12     | 0.01                | 0.11       |
| (1,967)  | 1:103:A:LYS:HB2  | 1:80:A:THR:HG22  | 7                   | 0.12     | 0.01                | 0.11       |
| (1,66)   | 1:9:A:THR:H      | 1:116:A:SER:HA   | 7                   | 0.12     | 0.01                | 0.12       |
| (1,1343) | 1:143:A:ILE:HG13 | 1:37:A:ALA:HA    | 6                   | 1.2      | 0.08                | 1.19       |
| (1,1308) | 1:71:A:ILE:HD11  | 1:83:A:CYS:HB3   | 6                   | 1.06     | 0.51                | 0.84       |
| (1,1308) | 1:71:A:ILE:HD12  | 1:83:A:CYS:HB3   | 6                   | 1.06     | 0.51                | 0.84       |
| (1,1308) | 1:71:A:ILE:HD13  | 1:83:A:CYS:HB3   | 6                   | 1.06     | 0.51                | 0.84       |
| (1,610)  | 1:149:A:ALA:H    | 1:152:A:LEU:HD23 | 6                   | 1.05     | 0.39                | 1.2        |
| (1,610)  | 1:149:A:ALA:H    | 1:152:A:LEU:HD21 | 6                   | 1.05     | 0.39                | 1.2        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,610)  | 1:149:A:ALA:H    | 1:152:A:LEU:HD22 | 6                   | 1.05     | 0.39                | 1.2        |
| (1,1132) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HG12 | 6                   | 1.05     | 0.02                | 1.06       |
| (1,1132) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HG12 | 6                   | 1.05     | 0.02                | 1.06       |
| (1,1132) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HG12 | 6                   | 1.05     | 0.02                | 1.06       |
| (1,321)  | 1:57:A:THR:H     | 1:38:A:ILE:HG12  | 6                   | 1.0      | 0.18                | 1.03       |
| (1,1023) | 1:17:A:ARG:HA    | 1:20:A:LYS:HE3   | 6                   | 0.92     | 0.59                | 0.71       |
| (1,1155) | 1:32:A:LYS:HA    | 1:32:A:LYS:HD3   | 6                   | 0.62     | 0.22                | 0.7        |
| (1,239)  | 1:42:A:GLU:H     | 1:55:A:LYS:HG2   | 6                   | 0.6      | 0.22                | 0.62       |
| (1,1038) | 1:18:A:LEU:HA    | 1:18:A:LEU:HD23  | 6                   | 0.59     | 0.07                | 0.56       |
| (1,1304) | 1:56:A:ILE:HD11  | 1:27:A:ASP:HA    | 6                   | 0.58     | 0.17                | 0.56       |
| (1,1304) | 1:56:A:ILE:HD13  | 1:27:A:ASP:HA    | 6                   | 0.58     | 0.17                | 0.56       |
| (1,1623) | 1:117:A:THR:HB   | 1:101:A:GLU:HB3  | 6                   | 0.55     | 0.15                | 0.52       |
| (1,1223) | 1:8:A:GLU:HG2    | 1:113:A:ILE:HG23 | 6                   | 0.46     | 0.14                | 0.47       |
| (1,1223) | 1:8:A:GLU:HG2    | 1:113:A:ILE:HG22 | 6                   | 0.46     | 0.14                | 0.47       |
| (1,216)  | 1:38:A:ILE:H     | 1:38:A:ILE:HG13  | 6                   | 0.44     | 0.06                | 0.41       |
| (1,1146) | 1:31:A:PRO:HG2   | 1:41:A:SER:HB2   | 6                   | 0.41     | 0.15                | 0.43       |
| (1,720)  | 1:128:A:ILE:H    | 1:128:A:ILE:HG13 | 6                   | 0.38     | 0.18                | 0.38       |
| (1,1512) | 1:84:A:THR:HG23  | 1:71:A:ILE:HA    | 6                   | 0.27     | 0.06                | 0.26       |
| (1,1512) | 1:84:A:THR:HG21  | 1:71:A:ILE:HA    | 6                   | 0.27     | 0.06                | 0.26       |
| (1,519)  | 1:97:A:LYS:H     | 1:91:A:ILE:HD12  | 6                   | 0.24     | 0.06                | 0.22       |
| (1,519)  | 1:97:A:LYS:H     | 1:91:A:ILE:HD13  | 6                   | 0.24     | 0.06                | 0.22       |
| (1,1762) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD22 | 6                   | 0.21     | 0.05                | 0.19       |
| (1,1762) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD23 | 6                   | 0.21     | 0.05                | 0.19       |
| (1,1762) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD21 | 6                   | 0.21     | 0.05                | 0.19       |
| (1,619)  | 1:110:A:GLY:H    | 1:109:A:ASP:HA   | 6                   | 0.17     | 0.03                | 0.18       |
| (1,614)  | 1:110:A:GLY:H    | 1:106:A:ALA:HB1  | 6                   | 0.17     | 0.07                | 0.14       |
| (1,614)  | 1:110:A:GLY:H    | 1:106:A:ALA:HB2  | 6                   | 0.17     | 0.07                | 0.14       |
| (1,614)  | 1:110:A:GLY:H    | 1:106:A:ALA:HB3  | 6                   | 0.17     | 0.07                | 0.14       |
| (1,373)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB3   | 6                   | 0.16     | 0.03                | 0.17       |
| (1,1211) | 1:38:A:ILE:HG21  | 1:38:A:ILE:HG12  | 6                   | 0.16     | 0.01                | 0.16       |
| (1,1211) | 1:38:A:ILE:HG23  | 1:38:A:ILE:HG12  | 6                   | 0.16     | 0.01                | 0.16       |
| (1,1211) | 1:38:A:ILE:HG22  | 1:38:A:ILE:HG12  | 6                   | 0.16     | 0.01                | 0.16       |
| (1,1685) | 1:16:A:ALA:HB3   | 1:20:A:LYS:HE3   | 5                   | 1.32     | 0.46                | 1.05       |
| (1,1685) | 1:16:A:ALA:HB1   | 1:20:A:LYS:HE3   | 5                   | 1.32     | 0.46                | 1.05       |
| (1,1685) | 1:16:A:ALA:HB2   | 1:20:A:LYS:HE3   | 5                   | 1.32     | 0.46                | 1.05       |
| (1,1095) | 1:29:A:LEU:HA    | 1:29:A:LEU:HD21  | 5                   | 1.16     | 0.12                | 1.16       |
| (1,1095) | 1:29:A:LEU:HA    | 1:29:A:LEU:HD22  | 5                   | 1.16     | 0.12                | 1.16       |
| (1,1095) | 1:29:A:LEU:HA    | 1:29:A:LEU:HD23  | 5                   | 1.16     | 0.12                | 1.16       |
| (1,1653) | 1:133:A:ILE:HG13 | 1:3:A:PHE:HD1    | 5                   | 1.08     | 0.38                | 1.18       |
| (1,1653) | 1:133:A:ILE:HG13 | 1:3:A:PHE:HD2    | 5                   | 1.08     | 0.38                | 1.18       |
| (1,26)   | 1:32:A:LYS:H     | 1:29:A:LEU:HD21  | 5                   | 0.91     | 0.14                | 0.89       |
| (1,26)   | 1:32:A:LYS:H     | 1:29:A:LEU:HD22  | 5                   | 0.91     | 0.14                | 0.89       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,26)   | 1:32:A:LYS:H     | 1:29:A:LEU:HD23  | 5                   | 0.91     | 0.14                | 0.89       |
| (1,1312) | 1:44:A:ILE:HG12  | 1:55:A:LYS:HE3   | 5                   | 0.81     | 0.52                | 0.86       |
| (1,1341) | 1:29:A:LEU:HD12  | 1:147:A:VAL:HA   | 5                   | 0.8      | 0.22                | 0.86       |
| (1,1341) | 1:29:A:LEU:HD11  | 1:147:A:VAL:HA   | 5                   | 0.8      | 0.22                | 0.86       |
| (1,1341) | 1:29:A:LEU:HD13  | 1:147:A:VAL:HA   | 5                   | 0.8      | 0.22                | 0.86       |
| (1,1326) | 1:85:A:LEU:HD22  | 1:85:A:LEU:HA    | 5                   | 0.73     | 0.29                | 0.72       |
| (1,1326) | 1:85:A:LEU:HD23  | 1:85:A:LEU:HA    | 5                   | 0.73     | 0.29                | 0.72       |
| (1,265)  | 1:46:A:GLY:H     | 1:43:A:ILE:HG23  | 5                   | 0.62     | 0.15                | 0.7        |
| (1,265)  | 1:46:A:GLY:H     | 1:43:A:ILE:HG22  | 5                   | 0.62     | 0.15                | 0.7        |
| (1,1607) | 1:111:A:GLY:HA3  | 1:14:A:THR:HG21  | 5                   | 0.4      | 0.18                | 0.37       |
| (1,1607) | 1:111:A:GLY:HA3  | 1:14:A:THR:HG22  | 5                   | 0.4      | 0.18                | 0.37       |
| (1,1571) | 1:128:A:ILE:HD12 | 1:120:A:TYR:HA   | 5                   | 0.39     | 0.12                | 0.45       |
| (1,1571) | 1:128:A:ILE:HD11 | 1:120:A:TYR:HA   | 5                   | 0.39     | 0.12                | 0.45       |
| (1,1571) | 1:128:A:ILE:HD13 | 1:120:A:TYR:HA   | 5                   | 0.39     | 0.12                | 0.45       |
| (1,1383) | 1:130:A:GLU:HG2  | 1:133:A:ILE:HG12 | 5                   | 0.37     | 0.17                | 0.34       |
| (1,1771) | 1:150:A:TYR:HA   | 1:154:A:ASN:HD22 | 5                   | 0.35     | 0.3                 | 0.27       |
| (1,1530) | 1:45:A:GLU:HA    | 1:43:A:ILE:HG23  | 5                   | 0.34     | 0.07                | 0.38       |
| (1,1530) | 1:45:A:GLU:HA    | 1:43:A:ILE:HG22  | 5                   | 0.34     | 0.07                | 0.38       |
| (1,1336) | 1:128:A:ILE:HD13 | 1:120:A:TYR:HB2  | 5                   | 0.34     | 0.16                | 0.38       |
| (1,1336) | 1:128:A:ILE:HD11 | 1:120:A:TYR:HB2  | 5                   | 0.34     | 0.16                | 0.38       |
| (3,153)  | 1:113:A:ILE:HD11 | 1:108:A:PRO:HG2  | 5                   | 0.29     | 0.13                | 0.28       |
| (3,153)  | 1:113:A:ILE:HD13 | 1:108:A:PRO:HG2  | 5                   | 0.29     | 0.13                | 0.28       |
| (3,153)  | 1:113:A:ILE:HD12 | 1:108:A:PRO:HG2  | 5                   | 0.29     | 0.13                | 0.28       |
| (1,562)  | 1:43:A:ILE:H     | 1:43:A:ILE:HD11  | 5                   | 0.26     | 0.01                | 0.26       |
| (1,1232) | 1:133:A:ILE:HG13 | 1:132:A:GLN:HB2  | 5                   | 0.24     | 0.15                | 0.19       |
| (3,9)    | 1:14:A:THR:H     | 1:111:A:GLY:HA2  | 5                   | 0.23     | 0.06                | 0.21       |
| (1,1626) | 1:118:A:SER:HB2  | 1:117:A:THR:HG22 | 5                   | 0.19     | 0.06                | 0.17       |
| (1,1626) | 1:118:A:SER:HB2  | 1:117:A:THR:HG23 | 5                   | 0.19     | 0.06                | 0.17       |
| (1,1626) | 1:118:A:SER:HB2  | 1:117:A:THR:HG21 | 5                   | 0.19     | 0.06                | 0.17       |
| (1,564)  | 1:104:A:LEU:H    | 1:104:A:LEU:HG   | 5                   | 0.12     | 0.02                | 0.12       |
| (1,1782) | 1:157:A:ALA:HA   | 1:155:A:PRO:HD2  | 5                   | 0.12     | 0.01                | 0.11       |
| (1,1200) | 1:38:A:ILE:HD12  | 1:38:A:ILE:HB    | 5                   | 0.11     | 0.01                | 0.12       |
| (1,1200) | 1:38:A:ILE:HD13  | 1:38:A:ILE:HB    | 5                   | 0.11     | 0.01                | 0.12       |
| (1,1200) | 1:38:A:ILE:HD11  | 1:38:A:ILE:HB    | 5                   | 0.11     | 0.01                | 0.12       |
| (4,64)   | 1:139:A:GLU:N    | 1:135:A:ALA:O    | 5                   | 0.11     | 0.01                | 0.1        |
| (1,894)  | 1:3:A:PHE:HB2    | 1:5:A:TYR:HD1    | 4                   | 1.08     | 0.28                | 1.09       |
| (1,894)  | 1:3:A:PHE:HB2    | 1:5:A:TYR:HD2    | 4                   | 1.08     | 0.28                | 1.09       |
| (1,1231) | 1:98:A:ILE:HG21  | 1:85:A:LEU:HD11  | 4                   | 0.73     | 0.44                | 0.74       |
| (1,1231) | 1:98:A:ILE:HG22  | 1:85:A:LEU:HD13  | 4                   | 0.73     | 0.44                | 0.74       |
| (1,1231) | 1:98:A:ILE:HG22  | 1:85:A:LEU:HD12  | 4                   | 0.73     | 0.44                | 0.74       |
| (1,1231) | 1:98:A:ILE:HG23  | 1:85:A:LEU:HD13  | 4                   | 0.73     | 0.44                | 0.74       |
| (1,828)  | 1:153:A:ALA:H    | 1:149:A:ALA:HB2  | 4                   | 0.66     | 0.24                | 0.68       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,828)  | 1:153:A:ALA:H    | 1:149:A:ALA:HB1  | 4                   | 0.66     | 0.24                | 0.68       |
| (1,828)  | 1:153:A:ALA:H    | 1:149:A:ALA:HB3  | 4                   | 0.66     | 0.24                | 0.68       |
| (3,121)  | 1:102:A:ILE:HD13 | 1:100:A:TYR:HB2  | 4                   | 0.6      | 0.09                | 0.58       |
| (3,121)  | 1:102:A:ILE:HD11 | 1:100:A:TYR:HB2  | 4                   | 0.6      | 0.09                | 0.58       |
| (1,1259) | 1:8:A:GLU:HG3    | 1:114:A:LEU:H    | 4                   | 0.58     | 0.17                | 0.62       |
| (1,162)  | 1:24:A:LEU:H     | 1:20:A:LYS:HB3   | 4                   | 0.51     | 0.23                | 0.54       |
| (1,1446) | 1:56:A:ILE:HD11  | 1:40:A:SER:HA    | 4                   | 0.48     | 0.12                | 0.48       |
| (1,1446) | 1:56:A:ILE:HD13  | 1:40:A:SER:HA    | 4                   | 0.48     | 0.12                | 0.48       |
| (1,493)  | 1:90:A:ALA:H     | 1:67:A:VAL:HG11  | 4                   | 0.44     | 0.33                | 0.26       |
| (1,493)  | 1:90:A:ALA:H     | 1:67:A:VAL:HG12  | 4                   | 0.44     | 0.33                | 0.26       |
| (1,535)  | 1:100:A:TYR:H    | 1:83:A:CYS:HB3   | 4                   | 0.43     | 0.17                | 0.41       |
| (1,58)   | 1:9:A:THR:H      | 1:8:A:GLU:HG3    | 4                   | 0.4      | 0.03                | 0.4        |
| (1,1091) | 1:27:A:ASP:HA    | 1:41:A:SER:HB2   | 4                   | 0.39     | 0.23                | 0.33       |
| (1,476)  | 1:86:A:ILE:H     | 1:86:A:ILE:HG22  | 4                   | 0.36     | 0.06                | 0.34       |
| (1,476)  | 1:86:A:ILE:H     | 1:86:A:ILE:HG21  | 4                   | 0.36     | 0.06                | 0.34       |
| (1,476)  | 1:86:A:ILE:H     | 1:86:A:ILE:HG23  | 4                   | 0.36     | 0.06                | 0.34       |
| (1,1043) | 1:18:A:LEU:HD23  | 1:22:A:PHE:HD2   | 4                   | 0.34     | 0.14                | 0.36       |
| (1,1043) | 1:18:A:LEU:HD23  | 1:22:A:PHE:HD1   | 4                   | 0.34     | 0.14                | 0.36       |
| (3,135)  | 1:115:A:LYS:HD3  | 1:8:A:GLU:HA     | 4                   | 0.32     | 0.12                | 0.36       |
| (1,1537) | 1:128:A:ILE:HD11 | 1:120:A:TYR:HB3  | 4                   | 0.21     | 0.09                | 0.21       |
| (1,1537) | 1:128:A:ILE:HD13 | 1:120:A:TYR:HB3  | 4                   | 0.21     | 0.09                | 0.21       |
| (1,195)  | 1:36:A:GLN:H     | 1:36:A:GLN:HB2   | 4                   | 0.17     | 0.02                | 0.17       |
| (1,334)  | 1:59:A:GLY:H     | 1:58:A:PHE:HB2   | 4                   | 0.17     | 0.06                | 0.15       |
| (1,1631) | 1:122:A:THR:HA   | 1:122:A:THR:HG23 | 4                   | 0.16     | 0.02                | 0.16       |
| (1,1631) | 1:122:A:THR:HA   | 1:122:A:THR:HG22 | 4                   | 0.16     | 0.02                | 0.16       |
| (1,1631) | 1:122:A:THR:HA   | 1:122:A:THR:HG21 | 4                   | 0.16     | 0.02                | 0.16       |
| (1,708)  | 1:122:A:THR:H    | 1:95:A:LEU:HA    | 4                   | 0.14     | 0.03                | 0.15       |
| (1,1432) | 1:69:A:HIS:HA    | 1:69:A:HIS:HD2   | 4                   | 0.14     | 0.03                | 0.15       |
| (1,1755) | 1:143:A:ILE:HA   | 1:146:A:ALA:H    | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1385) | 1:62:A:SER:HA    | 1:60:A:GLU:H     | 4                   | 0.12     | 0.01                | 0.12       |
| (1,98)   | 1:157:A:ALA:H    | 1:154:A:ASN:HA   | 4                   | 0.12     | 0.0                 | 0.12       |
| (1,79)   | 1:145:A:LYS:H    | 1:147:A:VAL:HG12 | 3                   | 2.16     | 0.03                | 2.17       |
| (1,79)   | 1:145:A:LYS:H    | 1:147:A:VAL:HG13 | 3                   | 2.16     | 0.03                | 2.17       |
| (1,804)  | 1:147:A:VAL:H    | 1:147:A:VAL:HG11 | 3                   | 1.13     | 0.02                | 1.14       |
| (1,804)  | 1:147:A:VAL:H    | 1:147:A:VAL:HG12 | 3                   | 1.13     | 0.02                | 1.14       |
| (1,187)  | 1:34:A:ALA:H     | 1:147:A:VAL:HG11 | 3                   | 0.97     | 0.16                | 0.95       |
| (1,187)  | 1:34:A:ALA:H     | 1:147:A:VAL:HG12 | 3                   | 0.97     | 0.16                | 0.95       |
| (1,1272) | 1:136:A:GLY:HA3  | 1:139:A:GLU:HB3  | 3                   | 0.96     | 0.58                | 1.19       |
| (1,94)   | 1:146:A:ALA:H    | 1:147:A:VAL:HG12 | 3                   | 0.92     | 0.03                | 0.93       |
| (1,136)  | 1:20:A:LYS:H     | 1:20:A:LYS:HB2   | 3                   | 0.77     | 0.0                 | 0.77       |
| (1,711)  | 1:123:A:LYS:H    | 1:95:A:LEU:HD13  | 3                   | 0.75     | 0.39                | 0.66       |
| (1,711)  | 1:123:A:LYS:H    | 1:95:A:LEU:HD12  | 3                   | 0.75     | 0.39                | 0.66       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1765) | 1:2:A:VAL:HG11   | 1:3:A:PHE:HA     | 3                   | 0.73     | 0.74                | 0.21       |
| (1,1765) | 1:2:A:VAL:HG13   | 1:3:A:PHE:HA     | 3                   | 0.73     | 0.74                | 0.21       |
| (1,1764) | 1:122:A:THR:HB   | 1:126:A:HIS:HB2  | 3                   | 0.58     | 0.02                | 0.58       |
| (1,1436) | 1:91:A:ILE:HA    | 1:91:A:ILE:HD12  | 3                   | 0.53     | 0.01                | 0.53       |
| (1,1436) | 1:91:A:ILE:HA    | 1:91:A:ILE:HD11  | 3                   | 0.53     | 0.01                | 0.53       |
| (1,1436) | 1:91:A:ILE:HA    | 1:91:A:ILE:HD13  | 3                   | 0.53     | 0.01                | 0.53       |
| (3,149)  | 1:4:A:THR:HG22   | 1:6:A:GLU:HB2    | 3                   | 0.42     | 0.4                 | 0.16       |
| (3,149)  | 1:4:A:THR:HG21   | 1:6:A:GLU:HB2    | 3                   | 0.42     | 0.4                 | 0.16       |
| (1,870)  | 1:145:A:LYS:H    | 1:144:A:PHE:HB2  | 3                   | 0.37     | 0.07                | 0.35       |
| (3,147)  | 1:80:A:THR:HA    | 1:103:A:LYS:HD2  | 3                   | 0.37     | 0.12                | 0.42       |
| (3,147)  | 1:80:A:THR:HA    | 1:103:A:LYS:HD3  | 3                   | 0.37     | 0.12                | 0.42       |
| (1,518)  | 1:97:A:LYS:H     | 1:85:A:LEU:HD12  | 3                   | 0.36     | 0.32                | 0.13       |
| (1,518)  | 1:97:A:LYS:H     | 1:85:A:LEU:HD11  | 3                   | 0.36     | 0.32                | 0.13       |
| (1,518)  | 1:97:A:LYS:H     | 1:85:A:LEU:HD13  | 3                   | 0.36     | 0.32                | 0.13       |
| (1,659)  | 1:115:A:LYS:H    | 1:115:A:LYS:HG2  | 3                   | 0.33     | 0.05                | 0.32       |
| (1,905)  | 1:4:A:THR:HG21   | 1:119:A:LYS:HB2  | 3                   | 0.31     | 0.14                | 0.29       |
| (1,1171) | 1:33:A:VAL:HG22  | 1:29:A:LEU:HB2   | 3                   | 0.29     | 0.12                | 0.36       |
| (1,1171) | 1:33:A:VAL:HG23  | 1:29:A:LEU:HB2   | 3                   | 0.29     | 0.12                | 0.36       |
| (3,157)  | 1:114:A:LEU:HD21 | 1:22:A:PHE:HD1   | 3                   | 0.27     | 0.13                | 0.3        |
| (3,157)  | 1:114:A:LEU:HD23 | 1:22:A:PHE:HD2   | 3                   | 0.27     | 0.13                | 0.3        |
| (3,157)  | 1:114:A:LEU:HD22 | 1:22:A:PHE:HE2   | 3                   | 0.27     | 0.13                | 0.3        |
| (1,1129) | 1:30:A:ILE:HG22  | 1:37:A:ALA:H     | 3                   | 0.27     | 0.14                | 0.2        |
| (1,1129) | 1:30:A:ILE:HG21  | 1:37:A:ALA:H     | 3                   | 0.27     | 0.14                | 0.2        |
| (1,1261) | 1:13:A:ILE:HB    | 1:18:A:LEU:HD22  | 3                   | 0.23     | 0.16                | 0.14       |
| (1,1261) | 1:13:A:ILE:HB    | 1:18:A:LEU:HD21  | 3                   | 0.23     | 0.16                | 0.14       |
| (1,702)  | 1:122:A:THR:H    | 1:128:A:ILE:HG13 | 3                   | 0.21     | 0.03                | 0.2        |
| (3,171)  | 1:156:A:ALA:HA   | 1:159:A:HIS:HB2  | 3                   | 0.2      | 0.02                | 0.2        |
| (3,171)  | 1:156:A:ALA:HA   | 1:159:A:HIS:HB3  | 3                   | 0.2      | 0.02                | 0.2        |
| (1,1025) | 1:128:A:ILE:HA   | 1:129:A:LYS:H    | 3                   | 0.2      | 0.03                | 0.21       |
| (1,347)  | 1:66:A:TYR:H     | 1:65:A:ASN:HB2   | 3                   | 0.16     | 0.02                | 0.17       |
| (1,1766) | 1:9:A:THR:HB     | 1:102:A:ILE:HG23 | 3                   | 0.16     | 0.04                | 0.14       |
| (1,1766) | 1:9:A:THR:HB     | 1:102:A:ILE:HG22 | 3                   | 0.16     | 0.04                | 0.14       |
| (1,1047) | 1:20:A:LYS:HA    | 1:23:A:VAL:HB    | 3                   | 0.15     | 0.01                | 0.16       |
| (1,1650) | 1:145:A:LYS:HA   | 1:148:A:GLU:HB3  | 3                   | 0.12     | 0.02                | 0.12       |
| (4,52)   | 1:113:A:ILE:N    | 1:105:A:VAL:O    | 3                   | 0.11     | 0.01                | 0.1        |
| (1,876)  | 1:132:A:GLN:HE22 | 1:132:A:GLN:HE21 | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,495)  | 1:91:A:ILE:H     | 1:85:A:LEU:HD13  | 2                   | 2.45     | 0.8                 | 2.45       |
| (1,1489) | 1:67:A:VAL:HG12  | 1:58:A:PHE:HZ    | 2                   | 1.92     | 0.27                | 1.92       |
| (1,1489) | 1:67:A:VAL:HG11  | 1:58:A:PHE:HZ    | 2                   | 1.92     | 0.27                | 1.92       |
| (1,1692) | 1:151:A:LEU:HA   | 1:151:A:LEU:HD22 | 2                   | 1.72     | 0.03                | 1.72       |
| (1,1692) | 1:151:A:LEU:HA   | 1:151:A:LEU:HD21 | 2                   | 1.72     | 0.03                | 1.72       |
| (1,1591) | 1:105:A:VAL:HG12 | 1:107:A:SER:HB2  | 2                   | 1.66     | 1.04                | 1.66       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1591) | 1:105:A:VAL:HG11 | 1:107:A:SER:HB2  | 2                   | 1.66     | 1.04                | 1.66       |
| (1,1241) | 1:102:A:ILE:HG13 | 1:116:A:SER:HB3  | 2                   | 0.94     | 0.17                | 0.94       |
| (3,85)   | 1:97:A:LYS:HE3   | 1:96:A:GLU:HG2   | 2                   | 0.9      | 0.18                | 0.9        |
| (3,85)   | 1:103:A:LYS:HE3  | 1:78:A:ASN:HB3   | 2                   | 0.9      | 0.18                | 0.9        |
| (1,365)  | 1:67:A:VAL:H     | 1:67:A:VAL:HG13  | 2                   | 0.89     | 0.3                 | 0.89       |
| (1,847)  | 1:17:A:ARG:HH11  | 1:151:A:LEU:HA   | 2                   | 0.88     | 0.38                | 0.88       |
| (1,1301) | 1:44:A:ILE:HD11  | 1:53:A:ILE:HA    | 2                   | 0.65     | 0.26                | 0.65       |
| (1,1301) | 1:44:A:ILE:HD12  | 1:53:A:ILE:HA    | 2                   | 0.65     | 0.26                | 0.65       |
| (1,1247) | 1:102:A:ILE:HG23 | 1:81:A:TYR:HB3   | 2                   | 0.63     | 0.09                | 0.63       |
| (1,1247) | 1:102:A:ILE:HG21 | 1:81:A:TYR:HB3   | 2                   | 0.63     | 0.09                | 0.63       |
| (1,965)  | 1:12:A:VAL:HG21  | 1:111:A:GLY:H    | 2                   | 0.62     | 0.46                | 0.62       |
| (1,1230) | 1:98:A:ILE:HG21  | 1:85:A:LEU:HG    | 2                   | 0.6      | 0.1                 | 0.6        |
| (1,1230) | 1:98:A:ILE:HG23  | 1:85:A:LEU:HG    | 2                   | 0.6      | 0.1                 | 0.6        |
| (1,1032) | 1:20:A:LYS:HE2   | 1:20:A:LYS:HB2   | 2                   | 0.48     | 0.06                | 0.48       |
| (1,1153) | 1:132:A:GLN:HA   | 1:132:A:GLN:HG2  | 2                   | 0.46     | 0.04                | 0.46       |
| (1,1246) | 1:102:A:ILE:HG23 | 1:81:A:TYR:HB2   | 2                   | 0.46     | 0.05                | 0.46       |
| (1,1246) | 1:102:A:ILE:HG21 | 1:81:A:TYR:HB2   | 2                   | 0.46     | 0.05                | 0.46       |
| (1,737)  | 1:132:A:GLN:H    | 1:132:A:GLN:HG2  | 2                   | 0.43     | 0.02                | 0.43       |
| (1,1243) | 1:53:A:ILE:HG12  | 1:45:A:GLU:HG3   | 2                   | 0.4      | 0.2                 | 0.4        |
| (1,1121) | 1:74:A:ILE:HD12  | 1:19:A:PHE:HD2   | 2                   | 0.4      | 0.28                | 0.4        |
| (1,1328) | 1:104:A:LEU:HD12 | 1:112:A:SER:HB3  | 2                   | 0.4      | 0.11                | 0.4        |
| (1,254)  | 1:45:A:GLU:H     | 1:53:A:ILE:HG12  | 2                   | 0.35     | 0.19                | 0.35       |
| (1,1234) | 1:133:A:ILE:HG13 | 1:128:A:ILE:HG21 | 2                   | 0.32     | 0.15                | 0.32       |
| (1,1234) | 1:133:A:ILE:HG13 | 1:128:A:ILE:HG22 | 2                   | 0.32     | 0.15                | 0.32       |
| (1,181)  | 1:33:A:VAL:H     | 1:147:A:VAL:HG11 | 2                   | 0.31     | 0.02                | 0.31       |
| (1,888)  | 1:2:A:VAL:HG13   | 1:121:A:HIS:HA   | 2                   | 0.24     | 0.01                | 0.24       |
| (3,103)  | 1:71:A:ILE:HG23  | 1:54:A:LYS:HE2   | 2                   | 0.22     | 0.02                | 0.22       |
| (3,103)  | 1:71:A:ILE:HG22  | 1:54:A:LYS:HE2   | 2                   | 0.22     | 0.02                | 0.22       |
| (1,364)  | 1:67:A:VAL:H     | 1:68:A:LYS:HG3   | 2                   | 0.22     | 0.04                | 0.22       |
| (1,40)   | 1:5:A:TYR:H      | 1:119:A:LYS:HG2  | 2                   | 0.21     | 0.1                 | 0.21       |
| (1,1131) | 1:91:A:ILE:HG21  | 1:96:A:GLU:H     | 2                   | 0.2      | 0.07                | 0.2        |
| (1,1131) | 1:91:A:ILE:HG22  | 1:96:A:GLU:H     | 2                   | 0.2      | 0.07                | 0.2        |
| (1,997)  | 1:82:A:ALA:HB1   | 1:73:A:GLU:HB3   | 2                   | 0.18     | 0.01                | 0.18       |
| (1,997)  | 1:82:A:ALA:HB2   | 1:73:A:GLU:HB3   | 2                   | 0.18     | 0.01                | 0.18       |
| (1,1699) | 1:153:A:ALA:HA   | 1:154:A:ASN:HA   | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1337) | 1:113:A:ILE:HD11 | 1:10:A:THR:HG22  | 2                   | 0.17     | 0.01                | 0.17       |
| (1,1337) | 1:113:A:ILE:HD12 | 1:10:A:THR:HG22  | 2                   | 0.17     | 0.01                | 0.17       |
| (1,1208) | 1:38:A:ILE:HG21  | 1:30:A:ILE:HB    | 2                   | 0.16     | 0.06                | 0.16       |
| (1,128)  | 1:18:A:LEU:H     | 1:13:A:ILE:HG23  | 2                   | 0.16     | 0.03                | 0.16       |
| (1,1456) | 1:127:A:GLU:HG3  | 1:127:A:GLU:H    | 2                   | 0.16     | 0.05                | 0.16       |
| (1,343)  | 1:63:A:GLN:HE22  | 1:63:A:GLN:HA    | 2                   | 0.15     | 0.04                | 0.15       |
| (1,837)  | 1:154:A:ASN:H    | 1:149:A:ALA:HA   | 2                   | 0.14     | 0.02                | 0.14       |

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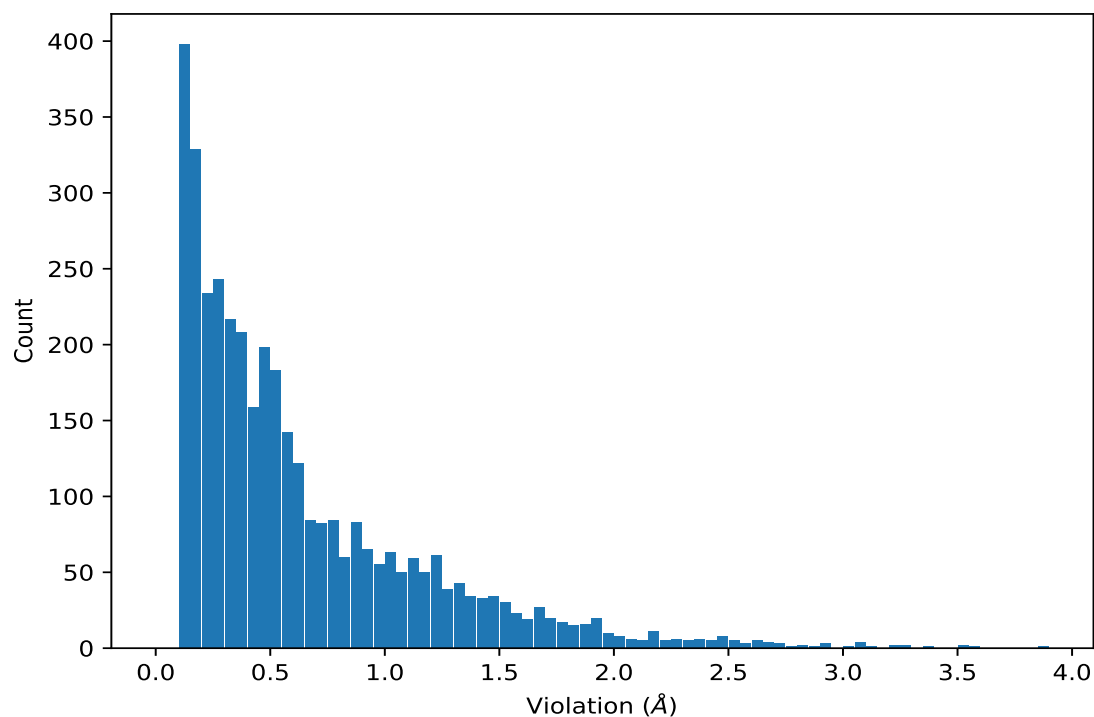
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1302) | 1:71:A:ILE:HD13 | 1:48:A:GLY:HA2  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1302) | 1:71:A:ILE:HD12 | 1:48:A:GLY:HA2  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1386) | 1:62:A:SER:HA   | 1:63:A:GLN:HE21 | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1239) | 1:43:A:ILE:HD11 | 1:43:A:ILE:HB   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1239) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HB   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1735) | 1:84:A:THR:HA   | 1:99:A:ALA:HA   | 2                   | 0.12     | 0.0                 | 0.12       |
| (4,32)   | 1:68:A:LYS:N    | 1:87:A:GLU:O    | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1281) | 1:155:A:PRO:HD3  | 1:151:A:LEU:HD21 | 13       | 3.9           |
| (1,1557) | 1:85:A:LEU:HD13  | 1:91:A:ILE:HG12  | 12       | 3.55          |
| (1,1589) | 1:105:A:VAL:HG13 | 1:107:A:SER:H    | 12       | 3.54          |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG23 | 12       | 3.52          |
| (1,1557) | 1:85:A:LEU:HD13  | 1:91:A:ILE:HG12  | 4        | 3.39          |
| (1,1183) | 1:34:A:ALA:HB1   | 1:147:A:VAL:HG11 | 2        | 3.26          |
| (1,495)  | 1:91:A:ILE:H     | 1:85:A:LEU:HD13  | 12       | 3.25          |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD21 | 20       | 3.24          |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD23 | 14       | 3.23          |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 19       | 3.11          |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 2        | 3.09          |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 13       | 3.07          |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD21 | 6        | 3.07          |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 16       | 3.06          |
| (1,1054) | 1:22:A:PHE:HA    | 1:29:A:LEU:HD13  | 3        | 3.04          |
| (1,1183) | 1:34:A:ALA:HB3   | 1:147:A:VAL:HG11 | 8        | 2.93          |
| (1,477)  | 1:87:A:GLU:H     | 1:67:A:VAL:HG23  | 12       | 2.93          |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 18       | 2.9           |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 9        | 2.85          |
| (1,1183) | 1:34:A:ALA:HB1   | 1:147:A:VAL:HG12 | 12       | 2.84          |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 7        | 2.8           |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD23 | 4        | 2.75          |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 2        | 2.72          |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 19       | 2.71          |
| (1,1591) | 1:105:A:VAL:HG12 | 1:107:A:SER:HB2  | 12       | 2.7           |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 18       | 2.69          |
| (1,890)  | 1:2:A:VAL:HG12   | 1:4:A:THR:HB     | 17       | 2.67          |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 14       | 2.66          |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 5        | 2.65          |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 4        | 2.64          |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 8        | 2.64          |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 12       | 2.62          |
| (1,849)  | 1:17:A:ARG:HH11  | 1:155:A:PRO:HG3  | 13       | 2.61          |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 3        | 2.6           |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD13 | 12       | 2.58          |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 9        | 2.57          |
| (1,477)  | 1:87:A:GLU:H     | 1:67:A:VAL:HG21  | 11       | 2.56          |
| (1,1071) | 1:23:A:VAL:HG11  | 1:22:A:PHE:HB3   | 3        | 2.54          |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 12       | 2.53          |
| (3,179)  | 1:148:A:GLU:HA   | 1:152:A:LEU:HD22 | 16       | 2.51          |
| (1,1281) | 1:155:A:PRO:HD3  | 1:151:A:LEU:HD22 | 9        | 2.51          |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 20       | 2.5           |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 13       | 2.49          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1071) | 1:23:A:VAL:HG11 | 1:22:A:PHE:HB3   | 7        | 2.48          |
| (1,1071) | 1:23:A:VAL:HG11 | 1:22:A:PHE:HB3   | 20       | 2.48          |
| (1,1562) | 1:145:A:LYS:HB2 | 1:142:A:GLY:HA3  | 10       | 2.47          |
| (1,1546) | 1:153:A:ALA:HB3 | 1:152:A:LEU:HA   | 7        | 2.47          |
| (1,1546) | 1:153:A:ALA:HB2 | 1:152:A:LEU:HA   | 18       | 2.47          |
| (1,1071) | 1:23:A:VAL:HG11 | 1:22:A:PHE:HB3   | 9        | 2.45          |
| (1,849)  | 1:17:A:ARG:HH11 | 1:155:A:PRO:HG3  | 19       | 2.45          |
| (1,1562) | 1:145:A:LYS:HB2 | 1:142:A:GLY:HA3  | 1        | 2.44          |
| (1,1703) | 1:154:A:ASN:HB3 | 1:17:A:ARG:HH11  | 8        | 2.43          |
| (1,1546) | 1:153:A:ALA:HB1 | 1:152:A:LEU:HA   | 3        | 2.42          |
| (1,1546) | 1:153:A:ALA:HB2 | 1:152:A:LEU:HA   | 15       | 2.42          |
| (1,849)  | 1:17:A:ARG:HH11 | 1:155:A:PRO:HG3  | 2        | 2.41          |
| (1,1071) | 1:23:A:VAL:HG13 | 1:22:A:PHE:HB3   | 16       | 2.39          |
| (1,1703) | 1:154:A:ASN:HB3 | 1:17:A:ARG:HH11  | 18       | 2.38          |
| (3,154)  | 1:85:A:LEU:HD22 | 1:83:A:CYS:HB3   | 11       | 2.37          |
| (1,1071) | 1:23:A:VAL:HG12 | 1:22:A:PHE:HB3   | 2        | 2.37          |
| (1,1546) | 1:153:A:ALA:HB1 | 1:152:A:LEU:HA   | 17       | 2.36          |
| (1,1546) | 1:153:A:ALA:HB1 | 1:152:A:LEU:HA   | 5        | 2.35          |
| (1,1546) | 1:153:A:ALA:HB2 | 1:152:A:LEU:HA   | 11       | 2.33          |
| (1,1546) | 1:153:A:ALA:HB1 | 1:152:A:LEU:HA   | 10       | 2.32          |
| (3,179)  | 1:148:A:GLU:HA  | 1:152:A:LEU:HD22 | 9        | 2.31          |
| (1,1071) | 1:23:A:VAL:HG11 | 1:22:A:PHE:HB3   | 5        | 2.3           |
| (1,107)  | 1:14:A:THR:H    | 1:12:A:VAL:HG12  | 3        | 2.3           |
| (1,1071) | 1:23:A:VAL:HG11 | 1:22:A:PHE:HB3   | 12       | 2.29          |
| (1,1071) | 1:23:A:VAL:HG13 | 1:22:A:PHE:HB3   | 13       | 2.28          |
| (1,1071) | 1:23:A:VAL:HG11 | 1:22:A:PHE:HB3   | 14       | 2.27          |
| (1,1071) | 1:23:A:VAL:HG13 | 1:22:A:PHE:HB3   | 18       | 2.26          |
| (1,957)  | 1:11:A:THR:HG23 | 1:112:A:SER:HB2  | 15       | 2.26          |
| (1,505)  | 1:96:A:GLU:H    | 1:85:A:LEU:HD11  | 12       | 2.25          |
| (1,1071) | 1:23:A:VAL:HG12 | 1:22:A:PHE:HB3   | 4        | 2.24          |
| (1,957)  | 1:11:A:THR:HG22 | 1:112:A:SER:HB2  | 2        | 2.23          |
| (1,957)  | 1:11:A:THR:HG22 | 1:112:A:SER:HB2  | 17       | 2.22          |
| (1,1071) | 1:23:A:VAL:HG12 | 1:22:A:PHE:HB3   | 1        | 2.2           |
| (1,1071) | 1:23:A:VAL:HG12 | 1:22:A:PHE:HB3   | 15       | 2.2           |
| (1,1701) | 1:153:A:ALA:HB3 | 1:154:A:ASN:HD22 | 6        | 2.19          |
| (1,1576) | 1:103:A:LYS:HE3 | 1:105:A:VAL:HG21 | 15       | 2.19          |
| (1,1111) | 1:30:A:ILE:HA   | 1:147:A:VAL:HG11 | 2        | 2.19          |
| (1,1546) | 1:153:A:ALA:HB2 | 1:152:A:LEU:HA   | 1        | 2.18          |
| (1,1489) | 1:67:A:VAL:HG12 | 1:58:A:PHE:HZ    | 11       | 2.18          |
| (1,79)   | 1:145:A:LYS:H   | 1:147:A:VAL:HG13 | 12       | 2.18          |
| (1,1071) | 1:23:A:VAL:HG11 | 1:22:A:PHE:HB3   | 6        | 2.17          |
| (1,79)   | 1:145:A:LYS:H   | 1:147:A:VAL:HG12 | 2        | 2.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1071) | 1:23:A:VAL:HG12  | 1:22:A:PHE:HB3   | 17       | 2.16          |
| (1,1071) | 1:23:A:VAL:HG11  | 1:22:A:PHE:HB3   | 19       | 2.16          |
| (1,957)  | 1:11:A:THR:HG23  | 1:112:A:SER:HB2  | 8        | 2.16          |
| (1,1310) | 1:44:A:ILE:HD11  | 1:68:A:LYS:HD2   | 19       | 2.14          |
| (1,1071) | 1:23:A:VAL:HG13  | 1:22:A:PHE:HB3   | 11       | 2.13          |
| (1,957)  | 1:11:A:THR:HG22  | 1:112:A:SER:HB2  | 1        | 2.13          |
| (1,79)   | 1:145:A:LYS:H    | 1:147:A:VAL:HG12 | 8        | 2.12          |
| (1,1071) | 1:23:A:VAL:HG12  | 1:22:A:PHE:HB3   | 8        | 2.11          |
| (1,1071) | 1:23:A:VAL:HG11  | 1:22:A:PHE:HB3   | 10       | 2.09          |
| (1,957)  | 1:11:A:THR:HG21  | 1:112:A:SER:HB2  | 9        | 2.09          |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 14       | 2.07          |
| (1,1701) | 1:153:A:ALA:HB1  | 1:154:A:ASN:HD22 | 13       | 2.06          |
| (1,310)  | 1:56:A:ILE:H     | 1:67:A:VAL:HG11  | 11       | 2.06          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 17       | 2.05          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 19       | 2.04          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 20       | 2.04          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 11       | 2.03          |
| (3,179)  | 1:148:A:GLU:HA   | 1:152:A:LEU:HD23 | 3        | 2.02          |
| (1,1310) | 1:44:A:ILE:HD13  | 1:68:A:LYS:HD2   | 4        | 2.02          |
| (3,154)  | 1:85:A:LEU:HD21  | 1:97:A:LYS:HE3   | 5        | 2.01          |
| (1,963)  | 1:12:A:VAL:HG12  | 1:13:A:ILE:HA    | 3        | 2.01          |
| (1,1054) | 1:22:A:PHE:HA    | 1:29:A:LEU:HD13  | 8        | 2.0           |
| (1,1310) | 1:44:A:ILE:HD13  | 1:68:A:LYS:HD2   | 15       | 1.99          |
| (1,904)  | 1:4:A:THR:HG22   | 1:6:A:GLU:HG3    | 20       | 1.99          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 13       | 1.98          |
| (1,957)  | 1:11:A:THR:HG23  | 1:112:A:SER:HB2  | 13       | 1.97          |
| (1,904)  | 1:4:A:THR:HG22   | 1:6:A:GLU:HG3    | 9        | 1.96          |
| (3,72)   | 1:11:A:THR:HG22  | 1:15:A:PRO:HA    | 10       | 1.95          |
| (1,1675) | 1:147:A:VAL:HG21 | 1:22:A:PHE:HB2   | 2        | 1.95          |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG23 | 16       | 1.95          |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG23 | 19       | 1.95          |
| (1,1310) | 1:44:A:ILE:HD13  | 1:68:A:LYS:HD2   | 2        | 1.95          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD12  | 10       | 1.94          |
| (1,1546) | 1:153:A:ALA:HB1  | 1:152:A:LEU:HA   | 6        | 1.94          |
| (1,1685) | 1:16:A:ALA:HB2   | 1:20:A:LYS:HE3   | 11       | 1.93          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 11       | 1.93          |
| (1,1310) | 1:44:A:ILE:HD12  | 1:68:A:LYS:HD2   | 11       | 1.93          |
| (1,1310) | 1:44:A:ILE:HD11  | 1:68:A:LYS:HD2   | 13       | 1.93          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 10       | 1.93          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 16       | 1.93          |
| (3,72)   | 1:11:A:THR:HG21  | 1:15:A:PRO:HA    | 9        | 1.92          |
| (1,1701) | 1:153:A:ALA:HB2  | 1:154:A:ASN:HD22 | 19       | 1.92          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB2   | 11       | 1.92          |
| (1,1531) | 1:19:A:PHE:HB2   | 1:20:A:LYS:HG2   | 11       | 1.92          |
| (1,1310) | 1:44:A:ILE:HD13  | 1:68:A:LYS:HD2   | 6        | 1.92          |
| (1,1308) | 1:71:A:ILE:HD13  | 1:83:A:CYS:HB3   | 6        | 1.92          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 12       | 1.92          |
| (1,1531) | 1:19:A:PHE:HB2   | 1:20:A:LYS:HG2   | 19       | 1.91          |
| (1,904)  | 1:4:A:THR:HG22   | 1:6:A:GLU:HG3    | 5        | 1.91          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 20       | 1.9           |
| (1,957)  | 1:11:A:THR:HG23  | 1:112:A:SER:HB2  | 5        | 1.9           |
| (1,904)  | 1:4:A:THR:HG22   | 1:6:A:GLU:HG3    | 11       | 1.9           |
| (1,1310) | 1:44:A:ILE:HD13  | 1:68:A:LYS:HD2   | 12       | 1.89          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 5        | 1.89          |
| (1,95)   | 1:13:A:ILE:H     | 1:12:A:VAL:HG11  | 3        | 1.89          |
| (3,72)   | 1:11:A:THR:HG21  | 1:15:A:PRO:HA    | 3        | 1.88          |
| (1,1701) | 1:153:A:ALA:HB1  | 1:154:A:ASN:HD22 | 1        | 1.88          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 2        | 1.88          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 4        | 1.88          |
| (1,1546) | 1:153:A:ALA:HB3  | 1:152:A:LEU:HA   | 4        | 1.88          |
| (1,1531) | 1:19:A:PHE:HB2   | 1:20:A:LYS:HG2   | 3        | 1.88          |
| (1,1531) | 1:19:A:PHE:HB2   | 1:20:A:LYS:HG2   | 10       | 1.88          |
| (1,1310) | 1:44:A:ILE:HD13  | 1:68:A:LYS:HD2   | 8        | 1.88          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG22  | 16       | 1.88          |
| (1,1310) | 1:44:A:ILE:HD11  | 1:68:A:LYS:HD2   | 5        | 1.86          |
| (1,904)  | 1:4:A:THR:HG21   | 1:6:A:GLU:HG3    | 3        | 1.86          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD12  | 1        | 1.85          |
| (1,1557) | 1:85:A:LEU:HD13  | 1:91:A:ILE:HG12  | 6        | 1.85          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB2   | 7        | 1.84          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 18       | 1.84          |
| (1,1701) | 1:153:A:ALA:HB3  | 1:154:A:ASN:HD22 | 16       | 1.83          |
| (1,1141) | 1:102:A:ILE:HG23 | 1:116:A:SER:HB3  | 17       | 1.83          |
| (1,904)  | 1:4:A:THR:HG21   | 1:6:A:GLU:HG3    | 16       | 1.83          |
| (1,1685) | 1:16:A:ALA:HB3   | 1:20:A:LYS:HE3   | 3        | 1.82          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 15       | 1.82          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 19       | 1.82          |
| (1,1531) | 1:19:A:PHE:HB2   | 1:20:A:LYS:HG2   | 15       | 1.82          |
| (1,1310) | 1:44:A:ILE:HD11  | 1:68:A:LYS:HD2   | 9        | 1.82          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 9        | 1.82          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD12  | 12       | 1.81          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 8        | 1.81          |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 10       | 1.8           |
| (1,1557) | 1:85:A:LEU:HD11  | 1:91:A:ILE:HG12  | 16       | 1.8           |
| (1,1765) | 1:2:A:VAL:HG11   | 1:3:A:PHE:HA     | 17       | 1.78          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1701) | 1:153:A:ALA:HB3  | 1:154:A:ASN:HD22 | 5        | 1.78          |
| (1,1557) | 1:85:A:LEU:HD12  | 1:91:A:ILE:HG12  | 11       | 1.77          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 6        | 1.77          |
| (1,1054) | 1:22:A:PHE:HA    | 1:29:A:LEU:HD12  | 5        | 1.77          |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 20       | 1.76          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 14       | 1.76          |
| (1,1141) | 1:102:A:ILE:HG23 | 1:116:A:SER:HB3  | 8        | 1.76          |
| (1,1030) | 1:55:A:LYS:HE3   | 1:44:A:ILE:HD13  | 6        | 1.76          |
| (1,1012) | 1:138:A:GLU:HB3  | 1:136:A:GLY:H    | 17       | 1.76          |
| (3,72)   | 1:11:A:THR:HG23  | 1:15:A:PRO:HA    | 12       | 1.75          |
| (1,1692) | 1:151:A:LEU:HA   | 1:151:A:LEU:HD22 | 9        | 1.75          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB1   | 9        | 1.75          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB1   | 14       | 1.75          |
| (1,1023) | 1:17:A:ARG:HA    | 1:20:A:LYS:HE3   | 8        | 1.75          |
| (1,1012) | 1:138:A:GLU:HB3  | 1:136:A:GLY:H    | 5        | 1.75          |
| (1,1012) | 1:138:A:GLU:HB3  | 1:136:A:GLY:H    | 13       | 1.75          |
| (3,72)   | 1:11:A:THR:HG21  | 1:15:A:PRO:HA    | 6        | 1.74          |
| (3,72)   | 1:11:A:THR:HG23  | 1:15:A:PRO:HA    | 15       | 1.74          |
| (3,14)   | 1:24:A:LEU:H     | 1:71:A:ILE:HD13  | 18       | 1.74          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG22  | 20       | 1.74          |
| (1,1012) | 1:138:A:GLU:HB3  | 1:136:A:GLY:H    | 1        | 1.74          |
| (1,1012) | 1:138:A:GLU:HB3  | 1:136:A:GLY:H    | 4        | 1.74          |
| (1,957)  | 1:11:A:THR:HG21  | 1:112:A:SER:HB2  | 19       | 1.74          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG21  | 11       | 1.73          |
| (1,1012) | 1:138:A:GLU:HB3  | 1:136:A:GLY:H    | 11       | 1.73          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 15       | 1.72          |
| (1,1012) | 1:138:A:GLU:HB3  | 1:136:A:GLY:H    | 10       | 1.72          |
| (1,1012) | 1:138:A:GLU:HB3  | 1:136:A:GLY:H    | 19       | 1.72          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 8        | 1.71          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD12  | 17       | 1.71          |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 19       | 1.71          |
| (1,1310) | 1:44:A:ILE:HD12  | 1:68:A:LYS:HD2   | 3        | 1.71          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 1        | 1.71          |
| (1,1012) | 1:138:A:GLU:HB3  | 1:136:A:GLY:H    | 3        | 1.7           |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 3        | 1.7           |
| (1,904)  | 1:4:A:THR:HG23   | 1:6:A:GLU:HG3    | 12       | 1.7           |
| (3,72)   | 1:11:A:THR:HG23  | 1:15:A:PRO:HA    | 8        | 1.69          |
| (1,1692) | 1:151:A:LEU:HA   | 1:151:A:LEU:HD21 | 13       | 1.69          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB3   | 5        | 1.68          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB2   | 20       | 1.68          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD13 | 5        | 1.68          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 1        | 1.67          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 5        | 1.67          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 6        | 1.67          |
| (1,1023) | 1:17:A:ARG:HA    | 1:20:A:LYS:HE3   | 18       | 1.67          |
| (1,943)  | 1:117:A:THR:HG21 | 1:101:A:GLU:HB3  | 16       | 1.67          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 4        | 1.66          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 10       | 1.66          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 11       | 1.66          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 17       | 1.66          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG22  | 4        | 1.66          |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 5        | 1.66          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 7        | 1.65          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 18       | 1.65          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 20       | 1.65          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD13  | 8        | 1.65          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD11  | 14       | 1.65          |
| (1,1489) | 1:67:A:VAL:HG11  | 1:58:A:PHE:HZ    | 12       | 1.65          |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 2        | 1.65          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 20       | 1.65          |
| (1,879)  | 1:2:A:VAL:HG23   | 1:121:A:HIS:HA   | 17       | 1.65          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 18       | 1.65          |
| (1,495)  | 1:91:A:ILE:H     | 1:85:A:LEU:HD13  | 4        | 1.65          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 12       | 1.64          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD12  | 7        | 1.64          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD12  | 4        | 1.63          |
| (1,1350) | 1:56:A:ILE:HG22  | 1:38:A:ILE:HG12  | 12       | 1.63          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG23  | 19       | 1.63          |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 14       | 1.63          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 14       | 1.62          |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 11       | 1.62          |
| (1,1551) | 1:114:A:LEU:HA   | 1:104:A:LEU:HD21 | 12       | 1.62          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG23  | 6        | 1.62          |
| (1,1682) | 1:149:A:ALA:HA   | 1:152:A:LEU:HD23 | 11       | 1.61          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD13  | 20       | 1.61          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB2   | 17       | 1.61          |
| (1,1126) | 1:139:A:GLU:HB2  | 1:136:A:GLY:H    | 14       | 1.61          |
| (3,72)   | 1:11:A:THR:HG23  | 1:15:A:PRO:HA    | 11       | 1.6           |
| (3,14)   | 1:24:A:LEU:H     | 1:151:A:LEU:HD13 | 12       | 1.6           |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG21 | 7        | 1.6           |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG22  | 3        | 1.6           |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG22  | 5        | 1.6           |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 16       | 1.59          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 19       | 1.59          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1150) | 1:31:A:PRO:HG2  | 1:30:A:ILE:HG23  | 20       | 1.59          |
| (1,1148) | 1:31:A:PRO:HG3  | 1:27:A:ASP:HB3   | 3        | 1.59          |
| (3,72)   | 1:11:A:THR:HG22 | 1:15:A:PRO:HA    | 18       | 1.58          |
| (1,1630) | 1:121:A:HIS:HB3 | 1:91:A:ILE:HD13  | 6        | 1.58          |
| (1,1562) | 1:145:A:LYS:HB2 | 1:142:A:GLY:HA3  | 16       | 1.58          |
| (1,1562) | 1:145:A:LYS:HB2 | 1:142:A:GLY:HA3  | 17       | 1.58          |
| (1,1126) | 1:139:A:GLU:HB2 | 1:136:A:GLY:H    | 19       | 1.58          |
| (1,1010) | 1:31:A:PRO:HD2  | 1:41:A:SER:HA    | 3        | 1.58          |
| (1,1010) | 1:31:A:PRO:HD2  | 1:41:A:SER:HA    | 9        | 1.58          |
| (1,886)  | 1:2:A:VAL:HG21  | 1:119:A:LYS:HD2  | 11       | 1.58          |
| (3,72)   | 1:11:A:THR:HG21 | 1:15:A:PRO:HA    | 17       | 1.57          |
| (3,14)   | 1:24:A:LEU:H    | 1:71:A:ILE:HD13  | 7        | 1.57          |
| (1,1150) | 1:31:A:PRO:HG2  | 1:30:A:ILE:HG22  | 8        | 1.57          |
| (1,849)  | 1:17:A:ARG:HH11 | 1:155:A:PRO:HG3  | 16       | 1.57          |
| (1,1576) | 1:103:A:LYS:HE3 | 1:105:A:VAL:HG21 | 3        | 1.56          |
| (1,1350) | 1:56:A:ILE:HG22 | 1:38:A:ILE:HG12  | 19       | 1.56          |
| (1,1680) | 1:149:A:ALA:HA  | 1:151:A:LEU:HB3  | 3        | 1.55          |
| (1,1625) | 1:118:A:SER:HB2 | 1:99:A:ALA:HB2   | 15       | 1.55          |
| (1,1242) | 1:53:A:ILE:HG12 | 1:44:A:ILE:HG23  | 10       | 1.55          |
| (1,1154) | 1:96:A:GLU:HA   | 1:123:A:LYS:HD3  | 12       | 1.55          |
| (1,1126) | 1:139:A:GLU:HB2 | 1:136:A:GLY:H    | 20       | 1.55          |
| (1,1630) | 1:121:A:HIS:HB3 | 1:91:A:ILE:HD12  | 3        | 1.54          |
| (1,1562) | 1:145:A:LYS:HB2 | 1:142:A:GLY:HA3  | 20       | 1.54          |
| (1,1546) | 1:153:A:ALA:HB2 | 1:152:A:LEU:HA   | 20       | 1.54          |
| (1,1350) | 1:56:A:ILE:HG21 | 1:38:A:ILE:HG12  | 5        | 1.54          |
| (1,1126) | 1:139:A:GLU:HB2 | 1:136:A:GLY:H    | 4        | 1.54          |
| (1,1054) | 1:22:A:PHE:HA   | 1:29:A:LEU:HD13  | 15       | 1.54          |
| (1,1051) | 1:148:A:GLU:HB3 | 1:144:A:PHE:HB3  | 16       | 1.54          |
| (1,1010) | 1:31:A:PRO:HD2  | 1:41:A:SER:HA    | 8        | 1.54          |
| (1,886)  | 1:2:A:VAL:HG21  | 1:119:A:LYS:HD2  | 5        | 1.54          |
| (1,1630) | 1:121:A:HIS:HB3 | 1:91:A:ILE:HD13  | 15       | 1.53          |
| (1,1308) | 1:71:A:ILE:HD11 | 1:83:A:CYS:HB3   | 4        | 1.53          |
| (1,1272) | 1:136:A:GLY:HA3 | 1:139:A:GLU:HB3  | 8        | 1.53          |
| (1,1148) | 1:31:A:PRO:HG3  | 1:27:A:ASP:HB3   | 4        | 1.53          |
| (1,1111) | 1:30:A:ILE:HA   | 1:147:A:VAL:HG12 | 12       | 1.53          |
| (1,1010) | 1:31:A:PRO:HD2  | 1:41:A:SER:HA    | 2        | 1.53          |
| (1,1701) | 1:153:A:ALA:HB1 | 1:154:A:ASN:HD22 | 20       | 1.52          |
| (1,1680) | 1:149:A:ALA:HA  | 1:151:A:LEU:HB3  | 2        | 1.52          |
| (1,1546) | 1:153:A:ALA:HB3 | 1:152:A:LEU:HA   | 14       | 1.52          |
| (1,1164) | 1:33:A:VAL:HA   | 1:150:A:TYR:HB3  | 9        | 1.52          |
| (1,1051) | 1:148:A:GLU:HB3 | 1:144:A:PHE:HB3  | 3        | 1.52          |
| (1,70)   | 1:10:A:THR:H    | 1:8:A:GLU:HG3    | 5        | 1.52          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG22  | 15       | 1.51          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 6        | 1.51          |
| (1,943)  | 1:117:A:THR:HG22 | 1:101:A:GLU:HB3  | 8        | 1.51          |
| (3,72)   | 1:11:A:THR:HG22  | 1:15:A:PRO:HA    | 16       | 1.5           |
| (1,1701) | 1:153:A:ALA:HB1  | 1:154:A:ASN:HD22 | 12       | 1.5           |
| (1,1675) | 1:147:A:VAL:HG21 | 1:22:A:PHE:HB2   | 12       | 1.5           |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD13  | 13       | 1.5           |
| (1,1154) | 1:96:A:GLU:HA    | 1:123:A:LYS:HD3  | 7        | 1.5           |
| (1,1126) | 1:139:A:GLU:HB2  | 1:136:A:GLY:H    | 15       | 1.5           |
| (3,14)   | 1:24:A:LEU:H     | 1:71:A:ILE:HD12  | 9        | 1.49          |
| (1,1653) | 1:133:A:ILE:HG13 | 1:3:A:PHE:HD1    | 19       | 1.49          |
| (1,1529) | 1:123:A:LYS:HA   | 1:96:A:GLU:HG2   | 10       | 1.49          |
| (1,1159) | 1:103:A:LYS:HG2  | 1:105:A:VAL:HA   | 3        | 1.49          |
| (1,1159) | 1:103:A:LYS:HG2  | 1:105:A:VAL:HA   | 7        | 1.49          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG22  | 2        | 1.49          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 1        | 1.49          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 4        | 1.49          |
| (1,70)   | 1:10:A:THR:H     | 1:8:A:GLU:HG3    | 16       | 1.49          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD11  | 19       | 1.48          |
| (1,1312) | 1:44:A:ILE:HG12  | 1:55:A:LYS:HE3   | 9        | 1.48          |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 3        | 1.48          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG21  | 12       | 1.48          |
| (1,1126) | 1:139:A:GLU:HB2  | 1:136:A:GLY:H    | 2        | 1.48          |
| (1,943)  | 1:117:A:THR:HG23 | 1:101:A:GLU:HB3  | 5        | 1.48          |
| (1,1310) | 1:44:A:ILE:HD13  | 1:68:A:LYS:HD2   | 20       | 1.47          |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 15       | 1.47          |
| (1,1159) | 1:103:A:LYS:HG2  | 1:105:A:VAL:HA   | 4        | 1.47          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD13 | 9        | 1.47          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 7        | 1.47          |
| (1,70)   | 1:10:A:THR:H     | 1:8:A:GLU:HG3    | 10       | 1.47          |
| (1,1159) | 1:103:A:LYS:HG2  | 1:105:A:VAL:HA   | 17       | 1.46          |
| (1,1126) | 1:139:A:GLU:HB2  | 1:136:A:GLY:H    | 11       | 1.46          |
| (1,886)  | 1:2:A:VAL:HG23   | 1:119:A:LYS:HD2  | 4        | 1.46          |
| (1,886)  | 1:2:A:VAL:HG23   | 1:119:A:LYS:HD2  | 19       | 1.46          |
| (1,886)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HD2  | 20       | 1.46          |
| (1,610)  | 1:149:A:ALA:H    | 1:152:A:LEU:HD21 | 20       | 1.46          |
| (1,70)   | 1:10:A:THR:H     | 1:8:A:GLU:HG3    | 4        | 1.46          |
| (1,70)   | 1:10:A:THR:H     | 1:8:A:GLU:HG3    | 20       | 1.46          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD11  | 11       | 1.45          |
| (1,1159) | 1:103:A:LYS:HG2  | 1:105:A:VAL:HA   | 14       | 1.45          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD13 | 18       | 1.45          |
| (1,581)  | 1:105:A:VAL:H    | 1:103:A:LYS:HG2  | 3        | 1.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,70)   | 1:10:A:THR:H     | 1:8:A:GLU:HG3    | 6        | 1.45          |
| (3,158)  | 1:118:A:SER:HB2  | 1:6:A:GLU:HB2    | 2        | 1.44          |
| (3,14)   | 1:24:A:LEU:H     | 1:104:A:LEU:HD11 | 17       | 1.44          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 5        | 1.44          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 4        | 1.44          |
| (1,943)  | 1:117:A:THR:HG22 | 1:101:A:GLU:HB3  | 13       | 1.44          |
| (1,894)  | 1:3:A:PHE:HB2    | 1:5:A:TYR:HD2    | 10       | 1.44          |
| (1,70)   | 1:10:A:THR:H     | 1:8:A:GLU:HG3    | 7        | 1.44          |
| (3,14)   | 1:24:A:LEU:H     | 1:151:A:LEU:HD12 | 16       | 1.43          |
| (1,1310) | 1:44:A:ILE:HD12  | 1:68:A:LYS:HD2   | 1        | 1.43          |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 10       | 1.43          |
| (1,1159) | 1:103:A:LYS:HG2  | 1:105:A:VAL:HA   | 15       | 1.43          |
| (1,1111) | 1:30:A:ILE:HA    | 1:147:A:VAL:HG11 | 8        | 1.43          |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 9        | 1.43          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 12       | 1.43          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 13       | 1.43          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 14       | 1.43          |
| (3,14)   | 1:24:A:LEU:H     | 1:104:A:LEU:HD22 | 11       | 1.42          |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 6        | 1.42          |
| (1,1562) | 1:145:A:LYS:HB2  | 1:142:A:GLY:HA3  | 15       | 1.42          |
| (1,1029) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD13 | 9        | 1.42          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 1        | 1.42          |
| (1,70)   | 1:10:A:THR:H     | 1:8:A:GLU:HG3    | 9        | 1.42          |
| (1,1529) | 1:123:A:LYS:HA   | 1:96:A:GLU:HG2   | 20       | 1.41          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 15       | 1.41          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 17       | 1.41          |
| (1,886)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HD2  | 6        | 1.41          |
| (1,70)   | 1:10:A:THR:H     | 1:8:A:GLU:HG3    | 13       | 1.41          |
| (1,1701) | 1:153:A:ALA:HB3  | 1:154:A:ASN:HD22 | 2        | 1.4           |
| (1,1529) | 1:123:A:LYS:HA   | 1:96:A:GLU:HG2   | 19       | 1.4           |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 1        | 1.4           |
| (1,1154) | 1:96:A:GLU:HA    | 1:123:A:LYS:HD3  | 4        | 1.4           |
| (1,1029) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD12 | 13       | 1.4           |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 19       | 1.4           |
| (3,72)   | 1:11:A:THR:HG23  | 1:15:A:PRO:HA    | 4        | 1.39          |
| (3,14)   | 1:24:A:LEU:H     | 1:71:A:ILE:HD11  | 13       | 1.39          |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 7        | 1.39          |
| (1,996)  | 1:82:A:ALA:HB2   | 1:73:A:GLU:HG3   | 7        | 1.39          |
| (1,610)  | 1:149:A:ALA:H    | 1:152:A:LEU:HD23 | 14       | 1.39          |
| (1,1529) | 1:123:A:LYS:HA   | 1:96:A:GLU:HG2   | 11       | 1.38          |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 1        | 1.38          |
| (3,72)   | 1:11:A:THR:HG23  | 1:15:A:PRO:HA    | 5        | 1.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,72)   | 1:11:A:THR:HG22  | 1:15:A:PRO:HA    | 14       | 1.37          |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 5        | 1.37          |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 14       | 1.37          |
| (1,886)  | 1:2:A:VAL:HG23   | 1:119:A:LYS:HD2  | 9        | 1.37          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 3        | 1.37          |
| (1,1618) | 1:114:A:LEU:HD22 | 1:9:A:THR:HB     | 20       | 1.36          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG21  | 1        | 1.36          |
| (1,1159) | 1:103:A:LYS:HG2  | 1:105:A:VAL:HA   | 20       | 1.36          |
| (1,1154) | 1:96:A:GLU:HA    | 1:123:A:LYS:HD3  | 5        | 1.36          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG21  | 7        | 1.36          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 15       | 1.36          |
| (1,1095) | 1:29:A:LEU:HA    | 1:29:A:LEU:HD21  | 3        | 1.36          |
| (1,1054) | 1:22:A:PHE:HA    | 1:29:A:LEU:HD13  | 11       | 1.36          |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 11       | 1.36          |
| (1,1019) | 1:146:A:ALA:HB1  | 1:142:A:GLY:HA3  | 16       | 1.36          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 18       | 1.36          |
| (1,904)  | 1:4:A:THR:HG22   | 1:6:A:GLU:HG3    | 6        | 1.36          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 4        | 1.36          |
| (1,70)   | 1:10:A:THR:H     | 1:8:A:GLU:HG3    | 1        | 1.36          |
| (3,154)  | 1:85:A:LEU:HD21  | 1:97:A:LYS:HE3   | 4        | 1.35          |
| (1,1231) | 1:98:A:ILE:HG22  | 1:85:A:LEU:HD12  | 4        | 1.35          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 11       | 1.35          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 2        | 1.35          |
| (1,884)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HG3  | 20       | 1.35          |
| (1,581)  | 1:105:A:VAL:H    | 1:103:A:LYS:HG2  | 4        | 1.35          |
| (1,581)  | 1:105:A:VAL:H    | 1:103:A:LYS:HG2  | 14       | 1.35          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 7        | 1.34          |
| (1,886)  | 1:2:A:VAL:HG22   | 1:119:A:LYS:HD2  | 2        | 1.34          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 16       | 1.34          |
| (1,70)   | 1:10:A:THR:H     | 1:8:A:GLU:HG3    | 18       | 1.34          |
| (3,141)  | 1:67:A:VAL:HG23  | 1:89:A:ASP:HB2   | 3        | 1.33          |
| (1,1529) | 1:123:A:LYS:HA   | 1:96:A:GLU:HG2   | 8        | 1.33          |
| (1,1343) | 1:143:A:ILE:HG13 | 1:37:A:ALA:HA    | 3        | 1.33          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 13       | 1.33          |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 4        | 1.33          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD11 | 1        | 1.33          |
| (1,1019) | 1:146:A:ALA:HB3  | 1:142:A:GLY:HA3  | 12       | 1.33          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 16       | 1.33          |
| (1,996)  | 1:82:A:ALA:HB2   | 1:73:A:GLU:HG3   | 11       | 1.33          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 13       | 1.33          |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG13 | 12       | 1.33          |
| (1,581)  | 1:105:A:VAL:H    | 1:103:A:LYS:HG2  | 15       | 1.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,14)   | 1:24:A:LEU:H     | 1:71:A:ILE:HD11  | 5        | 1.32          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD12  | 2        | 1.32          |
| (1,1529) | 1:123:A:LYS:HA   | 1:96:A:GLU:HG2   | 13       | 1.32          |
| (1,1019) | 1:146:A:ALA:HB3  | 1:142:A:GLY:HA3  | 13       | 1.32          |
| (1,996)  | 1:82:A:ALA:HB1   | 1:73:A:GLU:HG3   | 16       | 1.32          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 18       | 1.32          |
| (1,581)  | 1:105:A:VAL:H    | 1:103:A:LYS:HG2  | 7        | 1.32          |
| (1,1675) | 1:147:A:VAL:HG23 | 1:22:A:PHE:HB2   | 8        | 1.31          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD11  | 9        | 1.31          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG21  | 3        | 1.31          |
| (1,1019) | 1:146:A:ALA:HB1  | 1:142:A:GLY:HA3  | 1        | 1.31          |
| (1,1019) | 1:146:A:ALA:HB2  | 1:142:A:GLY:HA3  | 18       | 1.31          |
| (1,610)  | 1:149:A:ALA:H    | 1:152:A:LEU:HD21 | 6        | 1.31          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 6        | 1.31          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 10       | 1.31          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 12       | 1.31          |
| (1,581)  | 1:105:A:VAL:H    | 1:103:A:LYS:HG2  | 17       | 1.31          |
| (1,70)   | 1:10:A:THR:H     | 1:8:A:GLU:HG3    | 3        | 1.31          |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG22  | 13       | 1.3           |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 4        | 1.3           |
| (1,1612) | 1:112:A:SER:HB2  | 1:11:A:THR:HA    | 2        | 1.3           |
| (1,1529) | 1:123:A:LYS:HA   | 1:96:A:GLU:HG2   | 2        | 1.3           |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 11       | 1.3           |
| (1,1159) | 1:103:A:LYS:HG2  | 1:105:A:VAL:HA   | 10       | 1.3           |
| (1,1030) | 1:55:A:LYS:HE3   | 1:44:A:ILE:HD11  | 14       | 1.3           |
| (1,1019) | 1:146:A:ALA:HB1  | 1:142:A:GLY:HA3  | 9        | 1.3           |
| (1,1019) | 1:146:A:ALA:HB3  | 1:142:A:GLY:HA3  | 17       | 1.3           |
| (3,141)  | 1:67:A:VAL:HG22  | 1:89:A:ASP:HB3   | 5        | 1.29          |
| (1,1612) | 1:112:A:SER:HB2  | 1:11:A:THR:HA    | 17       | 1.29          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 2        | 1.29          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 20       | 1.29          |
| (1,1133) | 1:91:A:ILE:HG23  | 1:95:A:LEU:HB3   | 20       | 1.29          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 7        | 1.29          |
| (3,72)   | 1:11:A:THR:HG22  | 1:15:A:PRO:HA    | 1        | 1.28          |
| (1,1653) | 1:133:A:ILE:HG13 | 1:3:A:PHE:HD1    | 5        | 1.28          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD12  | 16       | 1.28          |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 8        | 1.28          |
| (1,1019) | 1:146:A:ALA:HB1  | 1:142:A:GLY:HA3  | 7        | 1.28          |
| (1,996)  | 1:82:A:ALA:HB2   | 1:73:A:GLU:HG3   | 4        | 1.28          |
| (1,943)  | 1:117:A:THR:HG21 | 1:101:A:GLU:HB3  | 18       | 1.28          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 7        | 1.28          |
| (3,179)  | 1:148:A:GLU:HA   | 1:152:A:LEU:HD22 | 11       | 1.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,132)  | 1:59:A:GLY:HA2   | 1:39:A:LYS:HB2   | 5        | 1.27          |
| (1,1529) | 1:123:A:LYS:HA   | 1:96:A:GLU:HG2   | 1        | 1.27          |
| (1,1154) | 1:96:A:GLU:HA    | 1:123:A:LYS:HD3  | 13       | 1.27          |
| (1,886)  | 1:2:A:VAL:HG22   | 1:119:A:LYS:HD2  | 7        | 1.27          |
| (1,847)  | 1:17:A:ARG:HH11  | 1:151:A:LEU:HA   | 18       | 1.27          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 11       | 1.27          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 20       | 1.27          |
| (3,158)  | 1:118:A:SER:HB2  | 1:6:A:GLU:HB2    | 1        | 1.26          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 8        | 1.26          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 14       | 1.26          |
| (1,1154) | 1:96:A:GLU:HA    | 1:123:A:LYS:HD3  | 10       | 1.26          |
| (1,711)  | 1:123:A:LYS:H    | 1:95:A:LEU:HD12  | 18       | 1.26          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 9        | 1.25          |
| (1,1680) | 1:149:A:ALA:HA   | 1:151:A:LEU:HB3  | 13       | 1.25          |
| (1,1612) | 1:112:A:SER:HB2  | 1:11:A:THR:HA    | 1        | 1.25          |
| (1,1573) | 1:113:A:ILE:HD13 | 1:106:A:ALA:HB3  | 2        | 1.25          |
| (1,1573) | 1:113:A:ILE:HD13 | 1:106:A:ALA:HB3  | 15       | 1.25          |
| (1,1343) | 1:143:A:ILE:HG13 | 1:37:A:ALA:HA    | 9        | 1.25          |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 4        | 1.25          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 16       | 1.25          |
| (1,1019) | 1:146:A:ALA:HB3  | 1:142:A:GLY:HA3  | 14       | 1.25          |
| (1,884)  | 1:2:A:VAL:HG22   | 1:119:A:LYS:HG3  | 2        | 1.25          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 11       | 1.25          |
| (1,70)   | 1:10:A:THR:H     | 1:8:A:GLU:HG3    | 19       | 1.25          |
| (3,14)   | 1:24:A:LEU:H     | 1:104:A:LEU:HD21 | 10       | 1.24          |
| (1,1618) | 1:114:A:LEU:HD22 | 1:9:A:THR:HB     | 12       | 1.24          |
| (1,1350) | 1:56:A:ILE:HG23  | 1:38:A:ILE:HG12  | 3        | 1.24          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 12       | 1.24          |
| (1,1312) | 1:44:A:ILE:HG12  | 1:55:A:LYS:HE3   | 14       | 1.24          |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD22 | 11       | 1.24          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 15       | 1.24          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 4        | 1.24          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 14       | 1.24          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 20       | 1.24          |
| (3,72)   | 1:11:A:THR:HG21  | 1:15:A:PRO:HA    | 2        | 1.23          |
| (1,1618) | 1:114:A:LEU:HD23 | 1:9:A:THR:HB     | 7        | 1.23          |
| (1,1612) | 1:112:A:SER:HB2  | 1:11:A:THR:HA    | 9        | 1.23          |
| (1,1612) | 1:112:A:SER:HB2  | 1:11:A:THR:HA    | 15       | 1.23          |
| (1,1573) | 1:113:A:ILE:HD11 | 1:106:A:ALA:HB3  | 11       | 1.23          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 20       | 1.23          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 12       | 1.23          |
| (1,1019) | 1:146:A:ALA:HB1  | 1:142:A:GLY:HA3  | 5        | 1.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1019) | 1:146:A:ALA:HB3  | 1:142:A:GLY:HA3  | 10       | 1.23          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 11       | 1.23          |
| (1,894)  | 1:3:A:PHE:HB2    | 1:5:A:TYR:HD2    | 18       | 1.23          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 2        | 1.23          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 18       | 1.23          |
| (3,141)  | 1:67:A:VAL:HG21  | 1:89:A:ASP:HB3   | 13       | 1.22          |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG23 | 8        | 1.22          |
| (1,1618) | 1:114:A:LEU:HD22 | 1:9:A:THR:HB     | 10       | 1.22          |
| (1,1573) | 1:113:A:ILE:HD13 | 1:106:A:ALA:HB2  | 8        | 1.22          |
| (1,1573) | 1:113:A:ILE:HD12 | 1:106:A:ALA:HB2  | 12       | 1.22          |
| (1,1573) | 1:113:A:ILE:HD11 | 1:106:A:ALA:HB3  | 17       | 1.22          |
| (1,1529) | 1:123:A:LYS:HA   | 1:96:A:GLU:HG2   | 15       | 1.22          |
| (1,1350) | 1:56:A:ILE:HG21  | 1:38:A:ILE:HG12  | 16       | 1.22          |
| (1,1343) | 1:143:A:ILE:HG13 | 1:37:A:ALA:HA    | 18       | 1.22          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 2        | 1.22          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 4        | 1.22          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 17       | 1.22          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 19       | 1.22          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG22  | 9        | 1.22          |
| (1,1030) | 1:55:A:LYS:HE3   | 1:44:A:ILE:HD12  | 11       | 1.22          |
| (1,1030) | 1:55:A:LYS:HE3   | 1:44:A:ILE:HD11  | 19       | 1.22          |
| (1,1019) | 1:146:A:ALA:HB1  | 1:142:A:GLY:HA3  | 2        | 1.22          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 1        | 1.22          |
| (3,179)  | 1:148:A:GLU:HA   | 1:18:A:LEU:HD22  | 1        | 1.21          |
| (3,141)  | 1:67:A:VAL:HG22  | 1:89:A:ASP:HB2   | 20       | 1.21          |
| (3,72)   | 1:11:A:THR:HG22  | 1:15:A:PRO:HA    | 7        | 1.21          |
| (1,1580) | 1:104:A:LEU:HA   | 1:104:A:LEU:HD21 | 12       | 1.21          |
| (1,1573) | 1:113:A:ILE:HD12 | 1:106:A:ALA:HB1  | 16       | 1.21          |
| (1,1529) | 1:123:A:LYS:HA   | 1:96:A:GLU:HG2   | 17       | 1.21          |
| (1,1350) | 1:56:A:ILE:HG23  | 1:38:A:ILE:HG12  | 7        | 1.21          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 7        | 1.21          |
| (1,1159) | 1:103:A:LYS:HG2  | 1:105:A:VAL:HA   | 2        | 1.21          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD12 | 11       | 1.21          |
| (1,1019) | 1:146:A:ALA:HB2  | 1:142:A:GLY:HA3  | 11       | 1.21          |
| (1,996)  | 1:82:A:ALA:HB2   | 1:73:A:GLU:HG3   | 6        | 1.21          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 20       | 1.21          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HB2    | 1        | 1.2           |
| (3,14)   | 1:24:A:LEU:H     | 1:71:A:ILE:HD13  | 1        | 1.2           |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 10       | 1.2           |
| (1,1095) | 1:29:A:LEU:HA    | 1:29:A:LEU:HD22  | 8        | 1.2           |
| (1,996)  | 1:82:A:ALA:HB1   | 1:73:A:GLU:HG3   | 1        | 1.2           |
| (1,581)  | 1:105:A:VAL:H    | 1:103:A:LYS:HG2  | 2        | 1.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,321)  | 1:57:A:THR:H     | 1:38:A:ILE:HG12  | 19       | 1.2           |
| (1,1618) | 1:114:A:LEU:HD21 | 1:9:A:THR:HB     | 6        | 1.19          |
| (1,1618) | 1:114:A:LEU:HD23 | 1:9:A:THR:HB     | 13       | 1.19          |
| (1,1272) | 1:136:A:GLY:HA3  | 1:139:A:GLU:HB3  | 12       | 1.19          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 6        | 1.19          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG22  | 11       | 1.19          |
| (1,1133) | 1:91:A:ILE:HG21  | 1:95:A:LEU:HB3   | 18       | 1.19          |
| (1,1019) | 1:146:A:ALA:HB1  | 1:142:A:GLY:HA3  | 8        | 1.19          |
| (1,1019) | 1:146:A:ALA:HB1  | 1:142:A:GLY:HA3  | 15       | 1.19          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 6        | 1.19          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 14       | 1.19          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 16       | 1.19          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 18       | 1.19          |
| (1,365)  | 1:67:A:VAL:H     | 1:67:A:VAL:HG13  | 12       | 1.19          |
| (3,141)  | 1:67:A:VAL:HG22  | 1:89:A:ASP:HB2   | 1        | 1.18          |
| (3,141)  | 1:67:A:VAL:HG22  | 1:89:A:ASP:HB3   | 2        | 1.18          |
| (3,14)   | 1:24:A:LEU:H     | 1:104:A:LEU:HD21 | 8        | 1.18          |
| (1,1653) | 1:133:A:ILE:HG13 | 1:3:A:PHE:HD2    | 6        | 1.18          |
| (1,1618) | 1:114:A:LEU:HD22 | 1:9:A:THR:HB     | 1        | 1.18          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 7        | 1.18          |
| (1,1019) | 1:146:A:ALA:HB1  | 1:142:A:GLY:HA3  | 3        | 1.18          |
| (1,1019) | 1:146:A:ALA:HB2  | 1:142:A:GLY:HA3  | 4        | 1.18          |
| (1,996)  | 1:82:A:ALA:HB3   | 1:73:A:GLU:HG3   | 10       | 1.18          |
| (1,996)  | 1:82:A:ALA:HB2   | 1:73:A:GLU:HG3   | 14       | 1.18          |
| (1,849)  | 1:17:A:ARG:HH11  | 1:155:A:PRO:HG3  | 1        | 1.18          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 3        | 1.18          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 7        | 1.18          |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 5        | 1.18          |
| (1,321)  | 1:57:A:THR:H     | 1:38:A:ILE:HG12  | 12       | 1.18          |
| (1,187)  | 1:34:A:ALA:H     | 1:147:A:VAL:HG11 | 2        | 1.18          |
| (1,1546) | 1:153:A:ALA:HB3  | 1:152:A:LEU:HA   | 8        | 1.17          |
| (1,1331) | 1:104:A:LEU:HD21 | 1:115:A:LYS:H    | 12       | 1.17          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 14       | 1.17          |
| (1,1019) | 1:146:A:ALA:HB2  | 1:142:A:GLY:HA3  | 19       | 1.17          |
| (1,943)  | 1:117:A:THR:HG23 | 1:101:A:GLU:HB3  | 7        | 1.17          |
| (1,885)  | 1:2:A:VAL:HG21   | 1:4:A:THR:HG21   | 14       | 1.17          |
| (1,849)  | 1:17:A:ARG:HH11  | 1:155:A:PRO:HG3  | 3        | 1.17          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 7        | 1.17          |
| (3,141)  | 1:67:A:VAL:HG21  | 1:89:A:ASP:HB3   | 14       | 1.16          |
| (1,1618) | 1:114:A:LEU:HD21 | 1:9:A:THR:HB     | 19       | 1.16          |
| (1,1529) | 1:123:A:LYS:HA   | 1:96:A:GLU:HG2   | 9        | 1.16          |
| (1,1343) | 1:143:A:ILE:HG13 | 1:37:A:ALA:HA    | 2        | 1.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1095) | 1:29:A:LEU:HA    | 1:29:A:LEU:HD22  | 11       | 1.16          |
| (1,996)  | 1:82:A:ALA:HB2   | 1:73:A:GLU:HG3   | 12       | 1.16          |
| (1,884)  | 1:2:A:VAL:HG22   | 1:119:A:LYS:HG3  | 7        | 1.16          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 7        | 1.16          |
| (1,26)   | 1:32:A:LYS:H     | 1:29:A:LEU:HD21  | 3        | 1.16          |
| (3,141)  | 1:67:A:VAL:HG22  | 1:89:A:ASP:HB3   | 6        | 1.15          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG23  | 4        | 1.15          |
| (1,804)  | 1:147:A:VAL:H    | 1:147:A:VAL:HG11 | 8        | 1.15          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 17       | 1.15          |
| (3,72)   | 1:11:A:THR:HG23  | 1:15:A:PRO:HA    | 13       | 1.14          |
| (1,1701) | 1:153:A:ALA:HB1  | 1:154:A:ASN:HD22 | 11       | 1.14          |
| (1,1618) | 1:114:A:LEU:HD22 | 1:9:A:THR:HB     | 17       | 1.14          |
| (1,1573) | 1:113:A:ILE:HD12 | 1:106:A:ALA:HB3  | 14       | 1.14          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 18       | 1.14          |
| (1,1343) | 1:143:A:ILE:HG13 | 1:37:A:ALA:HA    | 6        | 1.14          |
| (1,1341) | 1:29:A:LEU:HD13  | 1:147:A:VAL:HA   | 8        | 1.14          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 1        | 1.14          |
| (1,1159) | 1:103:A:LYS:HG2  | 1:105:A:VAL:HA   | 9        | 1.14          |
| (1,1019) | 1:146:A:ALA:HB3  | 1:142:A:GLY:HA3  | 6        | 1.14          |
| (1,804)  | 1:147:A:VAL:H    | 1:147:A:VAL:HG11 | 2        | 1.14          |
| (1,604)  | 1:107:A:SER:H    | 1:110:A:GLY:HA2  | 11       | 1.14          |
| (1,321)  | 1:57:A:THR:H     | 1:38:A:ILE:HG12  | 5        | 1.14          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 5        | 1.14          |
| (3,158)  | 1:118:A:SER:HB2  | 1:6:A:GLU:HB2    | 16       | 1.13          |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG21 | 4        | 1.13          |
| (1,1573) | 1:113:A:ILE:HD11 | 1:106:A:ALA:HB3  | 7        | 1.13          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 15       | 1.13          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 5        | 1.13          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG23  | 12       | 1.13          |
| (1,1133) | 1:91:A:ILE:HG23  | 1:95:A:LEU:HB3   | 16       | 1.13          |
| (1,1030) | 1:55:A:LYS:HE3   | 1:44:A:ILE:HD13  | 1        | 1.13          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 20       | 1.13          |
| (1,904)  | 1:4:A:THR:HG21   | 1:6:A:GLU:HG3    | 2        | 1.13          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 17       | 1.13          |
| (3,72)   | 1:11:A:THR:HG22  | 1:15:A:PRO:HA    | 20       | 1.12          |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG21  | 10       | 1.12          |
| (1,1618) | 1:114:A:LEU:HD23 | 1:9:A:THR:HB     | 11       | 1.12          |
| (1,1573) | 1:113:A:ILE:HD12 | 1:106:A:ALA:HB1  | 3        | 1.12          |
| (1,1573) | 1:113:A:ILE:HD11 | 1:106:A:ALA:HB3  | 20       | 1.12          |
| (1,1326) | 1:85:A:LEU:HD22  | 1:85:A:LEU:HA    | 5        | 1.12          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 18       | 1.12          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG23  | 16       | 1.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1019) | 1:146:A:ALA:HB1  | 1:142:A:GLY:HA3  | 20       | 1.12          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 20       | 1.12          |
| (1,375)  | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 7        | 1.12          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 1        | 1.12          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 3        | 1.12          |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG21  | 11       | 1.11          |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG23  | 15       | 1.11          |
| (1,1618) | 1:114:A:LEU:HD21 | 1:9:A:THR:HB     | 3        | 1.11          |
| (1,1618) | 1:114:A:LEU:HD23 | 1:9:A:THR:HB     | 4        | 1.11          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 15       | 1.11          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 19       | 1.11          |
| (1,1241) | 1:102:A:ILE:HG13 | 1:116:A:SER:HB3  | 17       | 1.11          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG22  | 14       | 1.11          |
| (1,996)  | 1:82:A:ALA:HB1   | 1:73:A:GLU:HG3   | 5        | 1.11          |
| (1,885)  | 1:2:A:VAL:HG21   | 1:4:A:THR:HG22   | 18       | 1.11          |
| (1,804)  | 1:147:A:VAL:H    | 1:147:A:VAL:HG12 | 12       | 1.11          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 10       | 1.11          |
| (3,158)  | 1:118:A:SER:HB2  | 1:6:A:GLU:HB2    | 3        | 1.1           |
| (1,1612) | 1:112:A:SER:HB2  | 1:11:A:THR:HA    | 5        | 1.1           |
| (1,1573) | 1:113:A:ILE:HD13 | 1:106:A:ALA:HB2  | 18       | 1.1           |
| (1,1546) | 1:153:A:ALA:HB3  | 1:152:A:LEU:HA   | 9        | 1.1           |
| (1,1536) | 1:68:A:LYS:HE2   | 1:44:A:ILE:HD12  | 7        | 1.1           |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD12  | 4        | 1.1           |
| (1,1233) | 1:133:A:ILE:HG13 | 1:128:A:ILE:HB   | 6        | 1.1           |
| (1,1133) | 1:91:A:ILE:HG22  | 1:95:A:LEU:HB3   | 13       | 1.1           |
| (1,904)  | 1:4:A:THR:HG22   | 1:6:A:GLU:HG3    | 4        | 1.1           |
| (1,1653) | 1:133:A:ILE:HG13 | 1:3:A:PHE:HD1    | 9        | 1.09          |
| (1,1618) | 1:114:A:LEU:HD21 | 1:9:A:THR:HB     | 14       | 1.09          |
| (1,1343) | 1:143:A:ILE:HG13 | 1:37:A:ALA:HA    | 4        | 1.09          |
| (1,1159) | 1:103:A:LYS:HG2  | 1:105:A:VAL:HA   | 19       | 1.09          |
| (1,1154) | 1:96:A:GLU:HA    | 1:123:A:LYS:HD3  | 3        | 1.09          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG21  | 10       | 1.09          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 3        | 1.09          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 11       | 1.09          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 2        | 1.09          |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG23 | 16       | 1.08          |
| (3,85)   | 1:103:A:LYS:HE3  | 1:78:A:ASN:HB3   | 18       | 1.08          |
| (1,1573) | 1:113:A:ILE:HD13 | 1:106:A:ALA:HB3  | 4        | 1.08          |
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 12       | 1.08          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG22  | 15       | 1.08          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 9        | 1.08          |
| (1,965)  | 1:12:A:VAL:HG21  | 1:111:A:GLY:H    | 3        | 1.08          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 6        | 1.08          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 10       | 1.08          |
| (1,610)  | 1:149:A:ALA:H    | 1:152:A:LEU:HD22 | 11       | 1.08          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 1        | 1.08          |
| (1,604)  | 1:107:A:SER:H    | 1:110:A:GLY:HA2  | 17       | 1.08          |
| (3,23)   | 1:45:A:GLU:H     | 1:43:A:ILE:HD13  | 19       | 1.07          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD11  | 5        | 1.07          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 7        | 1.07          |
| (1,1529) | 1:123:A:LYS:HA   | 1:96:A:GLU:HG2   | 3        | 1.07          |
| (1,1132) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HG12 | 6        | 1.07          |
| (1,1132) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HG12 | 18       | 1.07          |
| (3,158)  | 1:118:A:SER:HB2  | 1:6:A:GLU:HB2    | 12       | 1.06          |
| (3,141)  | 1:67:A:VAL:HG23  | 1:89:A:ASP:HB3   | 16       | 1.06          |
| (1,1612) | 1:112:A:SER:HB2  | 1:11:A:THR:HA    | 13       | 1.06          |
| (1,1612) | 1:112:A:SER:HB2  | 1:11:A:THR:HA    | 19       | 1.06          |
| (1,1308) | 1:71:A:ILE:HD13  | 1:83:A:CYS:HB3   | 9        | 1.06          |
| (1,1154) | 1:96:A:GLU:HA    | 1:123:A:LYS:HD3  | 8        | 1.06          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 14       | 1.06          |
| (1,1132) | 1:143:A:ILE:HG23 | 1:143:A:ILE:HG12 | 2        | 1.06          |
| (1,1095) | 1:29:A:LEU:HA    | 1:29:A:LEU:HD21  | 5        | 1.06          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 9        | 1.06          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 15       | 1.06          |
| (1,581)  | 1:105:A:VAL:H    | 1:103:A:LYS:HG2  | 20       | 1.06          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 4        | 1.06          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 11       | 1.06          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 16       | 1.06          |
| (3,141)  | 1:67:A:VAL:HG22  | 1:89:A:ASP:HB3   | 8        | 1.05          |
| (1,1685) | 1:16:A:ALA:HB2   | 1:20:A:LYS:HE3   | 10       | 1.05          |
| (1,1618) | 1:114:A:LEU:HD23 | 1:9:A:THR:HB     | 16       | 1.05          |
| (1,1573) | 1:113:A:ILE:HD13 | 1:106:A:ALA:HB3  | 10       | 1.05          |
| (1,1132) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HG12 | 4        | 1.05          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 15       | 1.05          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 10       | 1.05          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 18       | 1.05          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 18       | 1.04          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 3        | 1.04          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG11 | 5        | 1.04          |
| (1,1573) | 1:113:A:ILE:HD11 | 1:106:A:ALA:HB2  | 5        | 1.04          |
| (1,1573) | 1:113:A:ILE:HD11 | 1:106:A:ALA:HB2  | 6        | 1.04          |
| (1,1573) | 1:113:A:ILE:HD12 | 1:106:A:ALA:HB1  | 13       | 1.04          |
| (1,1573) | 1:113:A:ILE:HD12 | 1:106:A:ALA:HB3  | 19       | 1.04          |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG21  | 1        | 1.04          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 10       | 1.04          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG23  | 18       | 1.04          |
| (1,1132) | 1:143:A:ILE:HG22 | 1:143:A:ILE:HG12 | 9        | 1.04          |
| (1,1030) | 1:55:A:LYS:HE3   | 1:44:A:ILE:HD13  | 4        | 1.04          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 15       | 1.04          |
| (1,885)  | 1:2:A:VAL:HG22   | 1:4:A:THR:HG21   | 8        | 1.04          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 20       | 1.04          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB1   | 3        | 1.04          |
| (3,141)  | 1:67:A:VAL:HG21  | 1:89:A:ASP:HB3   | 15       | 1.03          |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG22 | 13       | 1.03          |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG23  | 9        | 1.03          |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG23  | 12       | 1.03          |
| (1,1678) | 1:134:A:LYS:HA   | 1:134:A:LYS:HD3  | 14       | 1.03          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 14       | 1.03          |
| (1,885)  | 1:2:A:VAL:HG21   | 1:4:A:THR:HG21   | 1        | 1.03          |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD23 | 17       | 1.03          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 8        | 1.03          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 13       | 1.03          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 15       | 1.03          |
| (3,141)  | 1:67:A:VAL:HG21  | 1:89:A:ASP:HB2   | 9        | 1.02          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 6        | 1.02          |
| (1,1573) | 1:113:A:ILE:HD13 | 1:106:A:ALA:HB1  | 1        | 1.02          |
| (1,1557) | 1:85:A:LEU:HD13  | 1:91:A:ILE:HG12  | 3        | 1.02          |
| (1,1546) | 1:153:A:ALA:HB2  | 1:152:A:LEU:HA   | 12       | 1.02          |
| (1,1536) | 1:68:A:LYS:HE2   | 1:44:A:ILE:HD12  | 18       | 1.02          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG22  | 13       | 1.02          |
| (1,1132) | 1:143:A:ILE:HG21 | 1:143:A:ILE:HG12 | 3        | 1.02          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 5        | 1.02          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD12  | 11       | 1.02          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB1   | 19       | 1.02          |
| (3,14)   | 1:24:A:LEU:H     | 1:71:A:ILE:HD11  | 19       | 1.01          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG12 | 19       | 1.01          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG21  | 1        | 1.01          |
| (1,1133) | 1:91:A:ILE:HG21  | 1:95:A:LEU:HB3   | 9        | 1.01          |
| (1,1030) | 1:55:A:LYS:HE3   | 1:44:A:ILE:HD12  | 9        | 1.01          |
| (1,604)  | 1:107:A:SER:H    | 1:110:A:GLY:HA2  | 2        | 1.01          |
| (1,604)  | 1:107:A:SER:H    | 1:110:A:GLY:HA2  | 12       | 1.01          |
| (1,581)  | 1:105:A:VAL:H    | 1:103:A:LYS:HG2  | 9        | 1.01          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 5        | 1.01          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB1   | 8        | 1.01          |
| (3,158)  | 1:118:A:SER:HB2  | 1:6:A:GLU:HB2    | 4        | 1.0           |
| (3,141)  | 1:67:A:VAL:HG23  | 1:89:A:ASP:HB2   | 19       | 1.0           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG23  | 8        | 1.0           |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 10       | 1.0           |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG11 | 8        | 1.0           |
| (1,1573) | 1:113:A:ILE:HD13 | 1:106:A:ALA:HB2  | 9        | 1.0           |
| (1,1557) | 1:85:A:LEU:HD13  | 1:91:A:ILE:HG12  | 17       | 1.0           |
| (1,1536) | 1:68:A:LYS:HE2   | 1:44:A:ILE:HD12  | 2        | 1.0           |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG22  | 6        | 1.0           |
| (1,1141) | 1:102:A:ILE:HG23 | 1:116:A:SER:HB3  | 20       | 1.0           |
| (1,1095) | 1:29:A:LEU:HA    | 1:29:A:LEU:HD23  | 15       | 1.0           |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 20       | 1.0           |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 17       | 1.0           |
| (1,604)  | 1:107:A:SER:H    | 1:110:A:GLY:HA2  | 10       | 1.0           |
| (1,493)  | 1:90:A:ALA:H     | 1:67:A:VAL:HG12  | 15       | 1.0           |
| (3,149)  | 1:4:A:THR:HG21   | 1:6:A:GLU:HB2    | 17       | 0.99          |
| (3,141)  | 1:67:A:VAL:HG22  | 1:89:A:ASP:HB2   | 17       | 0.99          |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 6        | 0.99          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG11 | 18       | 0.99          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 10       | 0.99          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 5        | 0.99          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 9        | 0.99          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 4        | 0.99          |
| (1,940)  | 1:10:A:THR:HG22  | 1:107:A:SER:HB2  | 14       | 0.99          |
| (1,875)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:H    | 6        | 0.99          |
| (1,604)  | 1:107:A:SER:H    | 1:110:A:GLY:HA2  | 15       | 0.99          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 1        | 0.99          |
| (1,239)  | 1:42:A:GLU:H     | 1:55:A:LYS:HG2   | 15       | 0.99          |
| (1,233)  | 1:70:A:ARG:HH22  | 1:70:A:ARG:HB2   | 19       | 0.99          |
| (3,72)   | 1:11:A:THR:HG21  | 1:15:A:PRO:HA    | 19       | 0.98          |
| (1,1612) | 1:112:A:SER:HB2  | 1:11:A:THR:HA    | 8        | 0.98          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG13 | 1        | 0.98          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 19       | 0.98          |
| (1,604)  | 1:107:A:SER:H    | 1:110:A:GLY:HA2  | 18       | 0.98          |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 11       | 0.98          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 13       | 0.98          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB3   | 5        | 0.98          |
| (1,1271) | 1:48:A:GLY:HA2   | 1:71:A:ILE:HG12  | 6        | 0.97          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 3        | 0.97          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 19       | 0.97          |
| (1,604)  | 1:107:A:SER:H    | 1:110:A:GLY:HA2  | 16       | 0.97          |
| (1,375)  | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 3        | 0.97          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 19       | 0.97          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB1   | 6        | 0.97          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,141)  | 1:67:A:VAL:HG23  | 1:89:A:ASP:HB3   | 18       | 0.96          |
| (1,1701) | 1:153:A:ALA:HB2  | 1:154:A:ASN:HD22 | 9        | 0.96          |
| (1,1618) | 1:114:A:LEU:HD21 | 1:9:A:THR:HB     | 2        | 0.96          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 10       | 0.96          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG12 | 9        | 0.96          |
| (1,1536) | 1:68:A:LYS:HE2   | 1:44:A:ILE:HD12  | 17       | 0.96          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 13       | 0.96          |
| (1,1233) | 1:133:A:ILE:HG13 | 1:128:A:ILE:HB   | 13       | 0.96          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD12 | 13       | 0.96          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 5        | 0.96          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 5        | 0.96          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 14       | 0.96          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB3   | 13       | 0.96          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 8        | 0.95          |
| (1,1150) | 1:31:A:PRO:HG2   | 1:30:A:ILE:HG22  | 17       | 0.95          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 10       | 0.95          |
| (1,894)  | 1:3:A:PHE:HB2    | 1:5:A:TYR:HD1    | 19       | 0.95          |
| (1,884)  | 1:2:A:VAL:HG22   | 1:119:A:LYS:HG3  | 3        | 0.95          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 9        | 0.95          |
| (1,581)  | 1:105:A:VAL:H    | 1:103:A:LYS:HG2  | 19       | 0.95          |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 7        | 0.95          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 2        | 0.95          |
| (1,187)  | 1:34:A:ALA:H     | 1:147:A:VAL:HG11 | 8        | 0.95          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB2   | 11       | 0.95          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB3   | 18       | 0.95          |
| (1,94)   | 1:146:A:ALA:H    | 1:147:A:VAL:HG12 | 2        | 0.95          |
| (1,1556) | 1:104:A:LEU:HD12 | 1:79:A:PHE:HB3   | 12       | 0.94          |
| (1,1543) | 1:156:A:ALA:HB3  | 1:154:A:ASN:HA   | 4        | 0.94          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 1        | 0.94          |
| (1,1326) | 1:85:A:LEU:HD22  | 1:85:A:LEU:HA    | 4        | 0.94          |
| (1,1204) | 1:38:A:ILE:HD13  | 1:58:A:PHE:HZ    | 5        | 0.94          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD12 | 19       | 0.94          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 5        | 0.94          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 9        | 0.94          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB2   | 12       | 0.94          |
| (1,133)  | 1:19:A:PHE:H     | 1:104:A:LEU:HD11 | 12       | 0.94          |
| (3,179)  | 1:148:A:GLU:HA   | 1:152:A:LEU:HD22 | 10       | 0.93          |
| (1,1771) | 1:150:A:TYR:HA   | 1:154:A:ASN:HD22 | 6        | 0.93          |
| (1,1685) | 1:16:A:ALA:HB1   | 1:20:A:LYS:HE3   | 18       | 0.93          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG13 | 10       | 0.93          |
| (1,1429) | 1:104:A:LEU:HD11 | 1:106:A:ALA:H    | 15       | 0.93          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 20       | 0.93          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1244) | 1:128:A:ILE:HG13 | 1:127:A:GLU:HB2  | 18       | 0.93          |
| (1,1141) | 1:102:A:ILE:HG22 | 1:116:A:SER:HB3  | 12       | 0.93          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 1        | 0.93          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 6        | 0.93          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 3        | 0.93          |
| (1,321)  | 1:57:A:THR:H     | 1:38:A:ILE:HG12  | 7        | 0.93          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB2   | 15       | 0.93          |
| (1,94)   | 1:146:A:ALA:H    | 1:147:A:VAL:HG12 | 8        | 0.93          |
| (1,26)   | 1:32:A:LYS:H     | 1:29:A:LEU:HD22  | 8        | 0.93          |
| (1,1630) | 1:121:A:HIS:HB3  | 1:91:A:ILE:HD11  | 18       | 0.92          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG13 | 7        | 0.92          |
| (1,1555) | 1:104:A:LEU:HD12 | 1:114:A:LEU:HA   | 20       | 0.92          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 5        | 0.92          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 11       | 0.92          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 7        | 0.92          |
| (1,996)  | 1:82:A:ALA:HB1   | 1:73:A:GLU:HG3   | 2        | 0.92          |
| (1,885)  | 1:2:A:VAL:HG23   | 1:4:A:THR:HG22   | 10       | 0.92          |
| (1,828)  | 1:153:A:ALA:H    | 1:149:A:ALA:HB1  | 2        | 0.92          |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD22 | 16       | 0.92          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 13       | 0.92          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 10       | 0.91          |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG23 | 5        | 0.91          |
| (1,1624) | 1:118:A:SER:HB2  | 1:119:A:LYS:HB2  | 20       | 0.91          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 12       | 0.91          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 16       | 0.91          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG11 | 11       | 0.91          |
| (1,1536) | 1:68:A:LYS:HE2   | 1:44:A:ILE:HD11  | 16       | 0.91          |
| (1,1524) | 1:20:A:LYS:HB3   | 1:19:A:PHE:HB2   | 7        | 0.91          |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG21  | 15       | 0.91          |
| (1,1304) | 1:56:A:ILE:HD11  | 1:27:A:ASP:HA    | 15       | 0.91          |
| (1,1301) | 1:44:A:ILE:HD12  | 1:53:A:ILE:HA    | 3        | 0.91          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 2        | 0.91          |
| (1,1233) | 1:133:A:ILE:HG13 | 1:128:A:ILE:HB   | 19       | 0.91          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 14       | 0.91          |
| (1,884)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HG3  | 5        | 0.91          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 8        | 0.91          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 9        | 0.91          |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 19       | 0.91          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 15       | 0.91          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 17       | 0.91          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB2   | 10       | 0.91          |
| (1,1678) | 1:134:A:LYS:HA   | 1:134:A:LYS:HD3  | 12       | 0.9           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 4        | 0.9           |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 14       | 0.9           |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 1        | 0.9           |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD23  | 3        | 0.9           |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 17       | 0.9           |
| (1,375)  | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 6        | 0.9           |
| (1,344)  | 1:64:A:PHE:H     | 1:57:A:THR:HG21  | 5        | 0.9           |
| (3,14)   | 1:24:A:LEU:H     | 1:71:A:ILE:HD12  | 20       | 0.89          |
| (1,1678) | 1:134:A:LYS:HA   | 1:134:A:LYS:HD3  | 20       | 0.89          |
| (1,1624) | 1:118:A:SER:HB2  | 1:119:A:LYS:HB2  | 7        | 0.89          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 4        | 0.89          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 13       | 0.89          |
| (1,1164) | 1:33:A:VAL:HA    | 1:150:A:TYR:HB3  | 3        | 0.89          |
| (1,1086) | 1:26:A:ALA:HA    | 1:29:A:LEU:HD13  | 3        | 0.89          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 12       | 0.89          |
| (1,996)  | 1:82:A:ALA:HB1   | 1:73:A:GLU:HG3   | 19       | 0.89          |
| (1,765)  | 1:139:A:GLU:H    | 1:138:A:GLU:HB3  | 1        | 0.89          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD11  | 7        | 0.89          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD22  | 6        | 0.89          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD21  | 13       | 0.89          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD21  | 14       | 0.89          |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 11       | 0.89          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 2        | 0.89          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 14       | 0.89          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB2   | 17       | 0.89          |
| (1,26)   | 1:32:A:LYS:H     | 1:29:A:LEU:HD22  | 11       | 0.89          |
| (3,14)   | 1:24:A:LEU:H     | 1:104:A:LEU:HD13 | 15       | 0.88          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG11 | 20       | 0.88          |
| (1,1524) | 1:20:A:LYS:HB3   | 1:19:A:PHE:HB2   | 16       | 0.88          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 20       | 0.88          |
| (1,1233) | 1:133:A:ILE:HG13 | 1:128:A:ILE:HB   | 3        | 0.88          |
| (1,996)  | 1:82:A:ALA:HB2   | 1:73:A:GLU:HG3   | 18       | 0.88          |
| (1,884)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HG3  | 12       | 0.88          |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD21 | 19       | 0.88          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 6        | 0.88          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 5        | 0.88          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 7        | 0.88          |
| (1,94)   | 1:146:A:ALA:H    | 1:147:A:VAL:HG12 | 12       | 0.88          |
| (3,179)  | 1:148:A:GLU:HA   | 1:152:A:LEU:HD22 | 12       | 0.87          |
| (3,141)  | 1:67:A:VAL:HG21  | 1:89:A:ASP:HB3   | 4        | 0.87          |
| (1,1623) | 1:117:A:THR:HB   | 1:101:A:GLU:HB3  | 16       | 0.87          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 6        | 0.87          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1541) | 1:143:A:ILE:HA   | 1:30:A:ILE:HG12  | 4        | 0.87          |
| (1,1536) | 1:68:A:LYS:HE2   | 1:44:A:ILE:HD11  | 14       | 0.87          |
| (1,1536) | 1:68:A:LYS:HE2   | 1:44:A:ILE:HD11  | 19       | 0.87          |
| (1,1524) | 1:20:A:LYS:HB3   | 1:19:A:PHE:HB2   | 5        | 0.87          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 5        | 0.87          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 16       | 0.87          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 18       | 0.87          |
| (1,996)  | 1:82:A:ALA:HB1   | 1:73:A:GLU:HG3   | 17       | 0.87          |
| (1,943)  | 1:117:A:THR:HG22 | 1:101:A:GLU:HB3  | 17       | 0.87          |
| (1,884)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HG3  | 11       | 0.87          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 8        | 0.87          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD21  | 9        | 0.87          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 12       | 0.87          |
| (3,58)   | 1:121:A:HIS:H    | 1:91:A:ILE:HD12  | 1        | 0.86          |
| (1,1701) | 1:153:A:ALA:HB2  | 1:154:A:ASN:HD22 | 4        | 0.86          |
| (1,1341) | 1:29:A:LEU:HD12  | 1:147:A:VAL:HA   | 11       | 0.86          |
| (1,1341) | 1:29:A:LEU:HD13  | 1:147:A:VAL:HA   | 15       | 0.86          |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG21  | 4        | 0.86          |
| (1,1312) | 1:44:A:ILE:HG12  | 1:55:A:LYS:HE3   | 6        | 0.86          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 10       | 0.86          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 11       | 0.86          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 17       | 0.86          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 19       | 0.86          |
| (1,885)  | 1:2:A:VAL:HG22   | 1:4:A:THR:HG21   | 9        | 0.86          |
| (1,828)  | 1:153:A:ALA:H    | 1:149:A:ALA:HB3  | 13       | 0.86          |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG21  | 16       | 0.85          |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 7        | 0.85          |
| (1,1701) | 1:153:A:ALA:HB1  | 1:154:A:ASN:HD22 | 15       | 0.85          |
| (1,1685) | 1:16:A:ALA:HB1   | 1:20:A:LYS:HE3   | 8        | 0.85          |
| (1,1557) | 1:85:A:LEU:HD13  | 1:91:A:ILE:HG12  | 15       | 0.85          |
| (1,1555) | 1:104:A:LEU:HD13 | 1:114:A:LEU:HA   | 7        | 0.85          |
| (1,1524) | 1:20:A:LYS:HB3   | 1:19:A:PHE:HB2   | 2        | 0.85          |
| (1,1524) | 1:20:A:LYS:HB3   | 1:19:A:PHE:HB2   | 13       | 0.85          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 17       | 0.85          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 19       | 0.85          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 17       | 0.85          |
| (1,1233) | 1:133:A:ILE:HG13 | 1:128:A:ILE:HB   | 5        | 0.85          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 11       | 0.85          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 17       | 0.85          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 12       | 0.85          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 6        | 0.85          |
| (1,375)  | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 19       | 0.85          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 9        | 0.85          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 17       | 0.85          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 9        | 0.85          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB2   | 2        | 0.85          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB3   | 7        | 0.85          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB3   | 9        | 0.85          |
| (3,14)   | 1:24:A:LEU:H     | 1:151:A:LEU:HD12 | 2        | 0.84          |
| (1,1701) | 1:153:A:ALA:HB2  | 1:154:A:ASN:HD22 | 14       | 0.84          |
| (1,1624) | 1:118:A:SER:HB2  | 1:119:A:LYS:HB2  | 11       | 0.84          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 3        | 0.84          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG11 | 15       | 0.84          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 13       | 0.84          |
| (1,996)  | 1:82:A:ALA:HB2   | 1:73:A:GLU:HG3   | 13       | 0.84          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 5        | 0.84          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD21  | 17       | 0.84          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB2   | 4        | 0.84          |
| (1,1624) | 1:118:A:SER:HB2  | 1:119:A:LYS:HB2  | 5        | 0.83          |
| (1,1555) | 1:104:A:LEU:HD12 | 1:114:A:LEU:HA   | 6        | 0.83          |
| (1,1524) | 1:20:A:LYS:HB3   | 1:19:A:PHE:HB2   | 8        | 0.83          |
| (1,1524) | 1:20:A:LYS:HB3   | 1:19:A:PHE:HB2   | 12       | 0.83          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 9        | 0.83          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 12       | 0.83          |
| (1,1010) | 1:31:A:PRO:HD2   | 1:41:A:SER:HA    | 10       | 0.83          |
| (1,996)  | 1:82:A:ALA:HB2   | 1:73:A:GLU:HG3   | 9        | 0.83          |
| (1,996)  | 1:82:A:ALA:HB1   | 1:73:A:GLU:HG3   | 15       | 0.83          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 8        | 0.83          |
| (1,885)  | 1:2:A:VAL:HG22   | 1:4:A:THR:HG21   | 4        | 0.83          |
| (1,616)  | 1:110:A:GLY:H    | 1:107:A:SER:HB3  | 14       | 0.83          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 13       | 0.83          |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 16       | 0.83          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB3   | 16       | 0.83          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 19       | 0.82          |
| (3,37)   | 1:82:A:ALA:H     | 1:70:A:ARG:HE    | 20       | 0.82          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 20       | 0.82          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG11 | 13       | 0.82          |
| (1,1541) | 1:143:A:ILE:HA   | 1:30:A:ILE:HG12  | 10       | 0.82          |
| (1,1524) | 1:20:A:LYS:HB3   | 1:19:A:PHE:HB2   | 18       | 0.82          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD11 | 8        | 0.82          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 8        | 0.82          |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD22 | 9        | 0.82          |
| (1,604)  | 1:107:A:SER:H    | 1:110:A:GLY:HA2  | 8        | 0.82          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 14       | 0.82          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 10       | 0.82          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 20       | 0.82          |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG21  | 18       | 0.81          |
| (1,1557) | 1:85:A:LEU:HD11  | 1:91:A:ILE:HG12  | 8        | 0.81          |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD12  | 6        | 0.81          |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG21  | 12       | 0.81          |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG23  | 13       | 0.81          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 12       | 0.81          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 13       | 0.81          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 15       | 0.81          |
| (1,1023) | 1:17:A:ARG:HA    | 1:20:A:LYS:HE3   | 10       | 0.81          |
| (1,996)  | 1:82:A:ALA:HB1   | 1:73:A:GLU:HG3   | 8        | 0.81          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 16       | 0.81          |
| (1,884)  | 1:2:A:VAL:HG23   | 1:119:A:LYS:HG3  | 9        | 0.81          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 9        | 0.81          |
| (1,518)  | 1:97:A:LYS:H     | 1:85:A:LEU:HD11  | 12       | 0.81          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 6        | 0.81          |
| (1,1595) | 1:16:A:ALA:HB3   | 1:19:A:PHE:HD2   | 12       | 0.8           |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 2        | 0.8           |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 18       | 0.8           |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG12 | 6        | 0.8           |
| (1,1543) | 1:156:A:ALA:HB2  | 1:154:A:ASN:HA   | 14       | 0.8           |
| (1,765)  | 1:139:A:GLU:H    | 1:138:A:GLU:HB3  | 4        | 0.8           |
| (1,26)   | 1:32:A:LYS:H     | 1:29:A:LEU:HD23  | 15       | 0.8           |
| (3,167)  | 1:146:A:ALA:HB1  | 1:35:A:PRO:HD2   | 10       | 0.79          |
| (3,167)  | 1:146:A:ALA:HB2  | 1:35:A:PRO:HD2   | 20       | 0.79          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 9        | 0.79          |
| (1,1536) | 1:68:A:LYS:HE2   | 1:44:A:ILE:HD12  | 10       | 0.79          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 4        | 0.79          |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG22  | 10       | 0.79          |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG22  | 11       | 0.79          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 3        | 0.79          |
| (1,1155) | 1:32:A:LYS:HA    | 1:32:A:LYS:HD3   | 4        | 0.79          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 19       | 0.79          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD22  | 16       | 0.79          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD21  | 19       | 0.79          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 6        | 0.79          |
| (1,344)  | 1:64:A:PHE:H     | 1:57:A:THR:HG22  | 15       | 0.79          |
| (1,321)  | 1:57:A:THR:H     | 1:38:A:ILE:HG12  | 16       | 0.79          |
| (1,310)  | 1:56:A:ILE:H     | 1:67:A:VAL:HG13  | 12       | 0.79          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 12       | 0.79          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 12       | 0.79          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,187)  | 1:34:A:ALA:H     | 1:147:A:VAL:HG12 | 12       | 0.79          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB2   | 1        | 0.79          |
| (1,162)  | 1:24:A:LEU:H     | 1:20:A:LYS:HB3   | 20       | 0.79          |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG22 | 14       | 0.78          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 16       | 0.78          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG13 | 16       | 0.78          |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD11  | 20       | 0.78          |
| (1,1231) | 1:98:A:ILE:HG21  | 1:85:A:LEU:HD11  | 12       | 0.78          |
| (1,903)  | 1:4:A:THR:HG21   | 1:5:A:TYR:HB2    | 17       | 0.78          |
| (1,765)  | 1:139:A:GLU:H    | 1:138:A:GLU:HB3  | 10       | 0.78          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 14       | 0.78          |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB3   | 14       | 0.78          |
| (3,179)  | 1:148:A:GLU:HA   | 1:18:A:LEU:HD23  | 2        | 0.77          |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 15       | 0.77          |
| (1,1624) | 1:118:A:SER:HB2  | 1:119:A:LYS:HB2  | 9        | 0.77          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG12 | 2        | 0.77          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG13 | 3        | 0.77          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG13 | 14       | 0.77          |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD13  | 5        | 0.77          |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD11  | 1        | 0.77          |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG21  | 20       | 0.77          |
| (1,1259) | 1:8:A:GLU:HG3    | 1:114:A:LEU:H    | 6        | 0.77          |
| (1,1241) | 1:102:A:ILE:HG13 | 1:116:A:SER:HB3  | 8        | 0.77          |
| (1,885)  | 1:2:A:VAL:HG21   | 1:4:A:THR:HG23   | 7        | 0.77          |
| (1,765)  | 1:139:A:GLU:H    | 1:138:A:GLU:HB3  | 11       | 0.77          |
| (1,765)  | 1:139:A:GLU:H    | 1:138:A:GLU:HB3  | 13       | 0.77          |
| (1,765)  | 1:139:A:GLU:H    | 1:138:A:GLU:HB3  | 17       | 0.77          |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 18       | 0.77          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 2        | 0.77          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 3        | 0.77          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 9        | 0.77          |
| (1,136)  | 1:20:A:LYS:H     | 1:20:A:LYS:HB2   | 9        | 0.77          |
| (1,136)  | 1:20:A:LYS:H     | 1:20:A:LYS:HB2   | 14       | 0.77          |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG23 | 20       | 0.76          |
| (1,1682) | 1:149:A:ALA:HA   | 1:152:A:LEU:HD23 | 17       | 0.76          |
| (1,1555) | 1:104:A:LEU:HD11 | 1:114:A:LEU:HA   | 14       | 0.76          |
| (1,1543) | 1:156:A:ALA:HB3  | 1:154:A:ASN:HA   | 6        | 0.76          |
| (1,1543) | 1:156:A:ALA:HB1  | 1:154:A:ASN:HA   | 8        | 0.76          |
| (1,1429) | 1:104:A:LEU:HD13 | 1:106:A:ALA:H    | 6        | 0.76          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 8        | 0.76          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 16       | 0.76          |
| (1,1233) | 1:133:A:ILE:HG13 | 1:128:A:ILE:HB   | 9        | 0.76          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,884)  | 1:2:A:VAL:HG23   | 1:119:A:LYS:HG3  | 19       | 0.76          |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 8        | 0.76          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 11       | 0.76          |
| (1,321)  | 1:57:A:THR:H     | 1:38:A:ILE:HG12  | 3        | 0.76          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 4        | 0.76          |
| (1,136)  | 1:20:A:LYS:H     | 1:20:A:LYS:HB2   | 20       | 0.76          |
| (1,26)   | 1:32:A:LYS:H     | 1:29:A:LEU:HD21  | 5        | 0.76          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 9        | 0.76          |
| (3,179)  | 1:148:A:GLU:HA   | 1:18:A:LEU:HD21  | 17       | 0.75          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 7        | 0.75          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 8        | 0.75          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 6        | 0.75          |
| (1,1541) | 1:143:A:ILE:HA   | 1:30:A:ILE:HG12  | 6        | 0.75          |
| (1,1524) | 1:20:A:LYS:HB3   | 1:19:A:PHE:HB2   | 1        | 0.75          |
| (1,1524) | 1:20:A:LYS:HB3   | 1:19:A:PHE:HB2   | 4        | 0.75          |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD11  | 2        | 0.75          |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG21  | 6        | 0.75          |
| (1,1271) | 1:48:A:GLY:HA2   | 1:71:A:ILE:HG12  | 8        | 0.75          |
| (1,1155) | 1:32:A:LYS:HA    | 1:32:A:LYS:HD3   | 9        | 0.75          |
| (1,886)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HD2  | 15       | 0.75          |
| (1,885)  | 1:2:A:VAL:HG23   | 1:4:A:THR:HG21   | 5        | 0.75          |
| (1,765)  | 1:139:A:GLU:H    | 1:138:A:GLU:HB3  | 5        | 0.75          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD12  | 4        | 0.75          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 13       | 0.75          |
| (3,121)  | 1:102:A:ILE:HD13 | 1:100:A:TYR:HB2  | 11       | 0.74          |
| (3,101)  | 1:74:A:ILE:HD13  | 1:49:A:GLY:HA2   | 6        | 0.74          |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG22 | 1        | 0.74          |
| (1,1607) | 1:111:A:GLY:HA3  | 1:14:A:THR:HG21  | 3        | 0.74          |
| (1,1555) | 1:104:A:LEU:HD12 | 1:114:A:LEU:HA   | 4        | 0.74          |
| (1,1524) | 1:20:A:LYS:HB3   | 1:19:A:PHE:HB2   | 17       | 0.74          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 18       | 0.74          |
| (1,1155) | 1:32:A:LYS:HA    | 1:32:A:LYS:HD3   | 1        | 0.74          |
| (1,1133) | 1:91:A:ILE:HG21  | 1:95:A:LEU:HB3   | 7        | 0.74          |
| (1,1091) | 1:27:A:ASP:HA    | 1:41:A:SER:HB2   | 1        | 0.74          |
| (1,1041) | 1:18:A:LEU:HB2   | 1:19:A:PHE:HB3   | 2        | 0.74          |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 9        | 0.74          |
| (1,375)  | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 20       | 0.74          |
| (1,265)  | 1:46:A:GLY:H     | 1:43:A:ILE:HG23  | 20       | 0.74          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 15       | 0.74          |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG21 | 7        | 0.73          |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG22 | 19       | 0.73          |
| (3,85)   | 1:97:A:LYS:HE3   | 1:96:A:GLU:HG2   | 10       | 0.73          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 8        | 0.73          |
| (1,1675) | 1:147:A:VAL:HG21 | 1:22:A:PHE:HB2   | 3        | 0.73          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG12 | 17       | 0.73          |
| (1,1524) | 1:20:A:LYS:HB3   | 1:19:A:PHE:HB2   | 6        | 0.73          |
| (1,1429) | 1:104:A:LEU:HD11 | 1:106:A:ALA:H    | 3        | 0.73          |
| (1,1429) | 1:104:A:LEU:HD12 | 1:106:A:ALA:H    | 14       | 0.73          |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG21  | 8        | 0.73          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 6        | 0.73          |
| (1,886)  | 1:2:A:VAL:HG22   | 1:119:A:LYS:HD2  | 3        | 0.73          |
| (1,882)  | 1:2:A:VAL:HG23   | 1:119:A:LYS:HE2  | 13       | 0.73          |
| (1,765)  | 1:139:A:GLU:H    | 1:138:A:GLU:HB3  | 3        | 0.73          |
| (1,765)  | 1:139:A:GLU:H    | 1:138:A:GLU:HB3  | 19       | 0.73          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD21  | 18       | 0.73          |
| (1,375)  | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 14       | 0.73          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 3        | 0.73          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 10       | 0.73          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 9        | 0.72          |
| (1,1582) | 1:104:A:LEU:HB3  | 1:105:A:VAL:HG12 | 4        | 0.72          |
| (1,1557) | 1:85:A:LEU:HD11  | 1:91:A:ILE:HG12  | 13       | 0.72          |
| (1,1557) | 1:85:A:LEU:HD13  | 1:91:A:ILE:HG12  | 19       | 0.72          |
| (1,1326) | 1:85:A:LEU:HD22  | 1:85:A:LEU:HA    | 11       | 0.72          |
| (1,1318) | 1:54:A:LYS:HA    | 1:53:A:ILE:HG22  | 3        | 0.72          |
| (1,1247) | 1:102:A:ILE:HG23 | 1:81:A:TYR:HB3   | 1        | 0.72          |
| (1,1159) | 1:103:A:LYS:HG2  | 1:105:A:VAL:HA   | 1        | 0.72          |
| (1,1038) | 1:18:A:LEU:HA    | 1:18:A:LEU:HD23  | 16       | 0.72          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 20       | 0.72          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 14       | 0.72          |
| (1,265)  | 1:46:A:GLY:H     | 1:43:A:ILE:HG23  | 6        | 0.72          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 2        | 0.72          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 4        | 0.72          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 6        | 0.72          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 19       | 0.72          |
| (1,1654) | 1:133:A:ILE:HG22 | 1:5:A:TYR:HB2    | 12       | 0.71          |
| (1,1636) | 1:122:A:THR:HG22 | 1:3:A:PHE:HE1    | 2        | 0.71          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 11       | 0.71          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 20       | 0.71          |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD12  | 4        | 0.71          |
| (1,1127) | 1:71:A:ILE:HG21  | 1:82:A:ALA:HA    | 4        | 0.71          |
| (1,1127) | 1:71:A:ILE:HG21  | 1:82:A:ALA:HA    | 6        | 0.71          |
| (1,581)  | 1:105:A:VAL:H    | 1:103:A:LYS:HG2  | 1        | 0.71          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD23  | 2        | 0.71          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 17       | 0.71          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 5        | 0.71          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 11       | 0.71          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 12       | 0.71          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 17       | 0.71          |
| (3,158)  | 1:118:A:SER:HB2  | 1:6:A:GLU:HB2    | 6        | 0.7           |
| (3,58)   | 1:121:A:HIS:H    | 1:91:A:ILE:HD11  | 13       | 0.7           |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11  | 3        | 0.7           |
| (1,1682) | 1:149:A:ALA:HA   | 1:152:A:LEU:HD22 | 10       | 0.7           |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 17       | 0.7           |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD11  | 11       | 0.7           |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 6        | 0.7           |
| (1,1230) | 1:98:A:ILE:HG21  | 1:85:A:LEU:HG    | 12       | 0.7           |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD11  | 7        | 0.7           |
| (1,894)  | 1:3:A:PHE:HB2    | 1:5:A:TYR:HD1    | 6        | 0.7           |
| (1,882)  | 1:2:A:VAL:HG22   | 1:119:A:LYS:HE2  | 2        | 0.7           |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 9        | 0.7           |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 17       | 0.7           |
| (1,565)  | 1:104:A:LEU:H    | 1:103:A:LYS:HG2  | 7        | 0.7           |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 15       | 0.7           |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 19       | 0.7           |
| (1,265)  | 1:46:A:GLY:H     | 1:43:A:ILE:HG22  | 4        | 0.7           |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 1        | 0.7           |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 9        | 0.69          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB2   | 3        | 0.69          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 4        | 0.69          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 4        | 0.69          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 11       | 0.69          |
| (1,1543) | 1:156:A:ALA:HB2  | 1:154:A:ASN:HA   | 7        | 0.69          |
| (1,1450) | 1:71:A:ILE:HG21  | 1:70:A:ARG:HE    | 3        | 0.69          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 16       | 0.69          |
| (1,1231) | 1:98:A:ILE:HG23  | 1:85:A:LEU:HD13  | 5        | 0.69          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 5        | 0.69          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 2        | 0.69          |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 18       | 0.69          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 14       | 0.69          |
| (3,141)  | 1:67:A:VAL:HG21  | 1:89:A:ASP:HB3   | 10       | 0.68          |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG21  | 7        | 0.68          |
| (1,1697) | 1:151:A:LEU:HD12 | 1:150:A:TYR:HD1  | 2        | 0.68          |
| (1,1660) | 1:143:A:ILE:HA   | 1:144:A:PHE:HD1  | 12       | 0.68          |
| (1,1654) | 1:133:A:ILE:HG23 | 1:5:A:TYR:HB2    | 9        | 0.68          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 7        | 0.68          |
| (1,1557) | 1:85:A:LEU:HD13  | 1:91:A:ILE:HG12  | 9        | 0.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1543) | 1:156:A:ALA:HB3  | 1:154:A:ASN:HA   | 13       | 0.68          |
| (1,1543) | 1:156:A:ALA:HB1  | 1:154:A:ASN:HA   | 17       | 0.68          |
| (1,1543) | 1:156:A:ALA:HB2  | 1:154:A:ASN:HA   | 20       | 0.68          |
| (1,1260) | 1:45:A:GLU:HG2   | 1:46:A:GLY:HA2   | 18       | 0.68          |
| (1,882)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HE2  | 12       | 0.68          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 6        | 0.68          |
| (1,849)  | 1:17:A:ARG:HH11  | 1:155:A:PRO:HG3  | 18       | 0.68          |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 7        | 0.68          |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 10       | 0.68          |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 14       | 0.68          |
| (1,610)  | 1:149:A:ALA:H    | 1:152:A:LEU:HD23 | 4        | 0.68          |
| (1,565)  | 1:104:A:LEU:H    | 1:103:A:LYS:HG2  | 10       | 0.68          |
| (1,565)  | 1:104:A:LEU:H    | 1:103:A:LYS:HG2  | 17       | 0.68          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 10       | 0.68          |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG21  | 5        | 0.67          |
| (1,1696) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HB   | 13       | 0.67          |
| (1,1595) | 1:16:A:ALA:HB1   | 1:19:A:PHE:HD1   | 13       | 0.67          |
| (1,1555) | 1:104:A:LEU:HD11 | 1:114:A:LEU:HA   | 15       | 0.67          |
| (1,1543) | 1:156:A:ALA:HB3  | 1:154:A:ASN:HA   | 9        | 0.67          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 17       | 0.67          |
| (1,1259) | 1:8:A:GLU:HG3    | 1:114:A:LEU:H    | 9        | 0.67          |
| (1,1223) | 1:8:A:GLU:HG2    | 1:113:A:ILE:HG22 | 11       | 0.67          |
| (1,1204) | 1:38:A:ILE:HD13  | 1:58:A:PHE:HZ    | 7        | 0.67          |
| (1,1204) | 1:38:A:ILE:HD13  | 1:58:A:PHE:HZ    | 15       | 0.67          |
| (1,1155) | 1:32:A:LYS:HA    | 1:32:A:LYS:HD3   | 7        | 0.67          |
| (1,1141) | 1:102:A:ILE:HG22 | 1:116:A:SER:HB3  | 1        | 0.67          |
| (1,1121) | 1:74:A:ILE:HD12  | 1:19:A:PHE:HD2   | 17       | 0.67          |
| (1,1084) | 1:26:A:ALA:HA    | 1:30:A:ILE:HG12  | 20       | 0.67          |
| (1,849)  | 1:17:A:ARG:HH11  | 1:155:A:PRO:HG3  | 8        | 0.67          |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD23 | 3        | 0.67          |
| (1,535)  | 1:100:A:TYR:H    | 1:83:A:CYS:HB3   | 11       | 0.67          |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 14       | 0.67          |
| (1,239)  | 1:42:A:GLU:H     | 1:55:A:LYS:HG2   | 18       | 0.67          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 5        | 0.66          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 11       | 0.66          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 14       | 0.66          |
| (1,1555) | 1:104:A:LEU:HD12 | 1:114:A:LEU:HA   | 16       | 0.66          |
| (1,1543) | 1:156:A:ALA:HB2  | 1:154:A:ASN:HA   | 16       | 0.66          |
| (1,1450) | 1:71:A:ILE:HG22  | 1:70:A:ARG:HE    | 13       | 0.66          |
| (1,1446) | 1:56:A:ILE:HD11  | 1:40:A:SER:HA    | 13       | 0.66          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 18       | 0.66          |
| (1,885)  | 1:2:A:VAL:HG23   | 1:4:A:THR:HG22   | 12       | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,711)  | 1:123:A:LYS:H    | 1:95:A:LEU:HD13  | 7        | 0.66          |
| (1,606)  | 1:107:A:SER:H    | 1:15:A:PRO:HG2   | 19       | 0.66          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 18       | 0.66          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 8        | 0.66          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 8        | 0.66          |
| (1,239)  | 1:42:A:GLU:H     | 1:55:A:LYS:HG2   | 13       | 0.66          |
| (1,233)  | 1:70:A:ARG:HH22  | 1:70:A:ARG:HB2   | 13       | 0.66          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 20       | 0.66          |
| (3,179)  | 1:148:A:GLU:HA   | 1:18:A:LEU:HD21  | 20       | 0.65          |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG23 | 10       | 0.65          |
| (1,1595) | 1:16:A:ALA:HB2   | 1:19:A:PHE:HD1   | 2        | 0.65          |
| (1,1595) | 1:16:A:ALA:HB1   | 1:19:A:PHE:HD1   | 15       | 0.65          |
| (1,1555) | 1:104:A:LEU:HD13 | 1:114:A:LEU:HA   | 3        | 0.65          |
| (1,1148) | 1:31:A:PRO:HG3   | 1:27:A:ASP:HB3   | 7        | 0.65          |
| (1,885)  | 1:2:A:VAL:HG23   | 1:4:A:THR:HG21   | 6        | 0.65          |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 3        | 0.65          |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 18       | 0.65          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD22  | 20       | 0.65          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD12  | 1        | 0.65          |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 8        | 0.65          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 7        | 0.65          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 8        | 0.65          |
| (3,179)  | 1:148:A:GLU:HA   | 1:18:A:LEU:HD23  | 4        | 0.64          |
| (3,121)  | 1:102:A:ILE:HD13 | 1:100:A:TYR:HB2  | 18       | 0.64          |
| (1,1654) | 1:133:A:ILE:HG23 | 1:5:A:TYR:HB2    | 13       | 0.64          |
| (1,1595) | 1:16:A:ALA:HB3   | 1:19:A:PHE:HD1   | 1        | 0.64          |
| (1,1595) | 1:16:A:ALA:HB3   | 1:19:A:PHE:HD2   | 6        | 0.64          |
| (1,1595) | 1:16:A:ALA:HB2   | 1:19:A:PHE:HD2   | 10       | 0.64          |
| (1,1595) | 1:16:A:ALA:HB1   | 1:19:A:PHE:HD2   | 18       | 0.64          |
| (1,1595) | 1:16:A:ALA:HB3   | 1:19:A:PHE:HD1   | 19       | 0.64          |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD12  | 17       | 0.64          |
| (1,1555) | 1:104:A:LEU:HD11 | 1:114:A:LEU:HA   | 17       | 0.64          |
| (1,1340) | 1:128:A:ILE:HD13 | 1:98:A:ILE:HG23  | 7        | 0.64          |
| (1,1127) | 1:71:A:ILE:HG22  | 1:82:A:ALA:HA    | 12       | 0.64          |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD11  | 13       | 0.64          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 4        | 0.64          |
| (1,955)  | 1:11:A:THR:HG23  | 1:9:A:THR:HA     | 1        | 0.64          |
| (1,955)  | 1:11:A:THR:HG22  | 1:9:A:THR:HA     | 2        | 0.64          |
| (1,885)  | 1:2:A:VAL:HG21   | 1:4:A:THR:HG23   | 16       | 0.64          |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3  | 10       | 0.64          |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 13       | 0.64          |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 14       | 0.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,179)  | 1:148:A:GLU:HA   | 1:18:A:LEU:HD22  | 5        | 0.63          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 16       | 0.63          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 20       | 0.63          |
| (1,1595) | 1:16:A:ALA:HB2   | 1:19:A:PHE:HD2   | 5        | 0.63          |
| (1,1543) | 1:156:A:ALA:HB2  | 1:154:A:ASN:HA   | 10       | 0.63          |
| (1,1450) | 1:71:A:ILE:HG23  | 1:70:A:ARG:HE    | 12       | 0.63          |
| (1,1450) | 1:71:A:ILE:HG23  | 1:70:A:ARG:HE    | 18       | 0.63          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 9        | 0.63          |
| (1,1326) | 1:85:A:LEU:HD23  | 1:85:A:LEU:HA    | 12       | 0.63          |
| (1,1238) | 1:43:A:ILE:HD13  | 1:48:A:GLY:HA2   | 3        | 0.63          |
| (1,1155) | 1:32:A:LYS:HA    | 1:32:A:LYS:HD3   | 13       | 0.63          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD11 | 3        | 0.63          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD13 | 20       | 0.63          |
| (1,960)  | 1:12:A:VAL:HA    | 1:12:A:VAL:HG22  | 3        | 0.63          |
| (1,849)  | 1:17:A:ARG:HH11  | 1:155:A:PRO:HG3  | 12       | 0.63          |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 12       | 0.63          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG23  | 12       | 0.63          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 16       | 0.63          |
| (1,565)  | 1:104:A:LEU:H    | 1:103:A:LYS:HG2  | 2        | 0.63          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD11  | 20       | 0.63          |
| (1,344)  | 1:64:A:PHE:H     | 1:57:A:THR:HG21  | 18       | 0.63          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 13       | 0.63          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 4        | 0.62          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HB2    | 14       | 0.62          |
| (3,14)   | 1:24:A:LEU:H     | 1:71:A:ILE:HD11  | 3        | 0.62          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 12       | 0.62          |
| (1,1654) | 1:133:A:ILE:HG22 | 1:5:A:TYR:HB2    | 15       | 0.62          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB3   | 19       | 0.62          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 18       | 0.62          |
| (1,1595) | 1:16:A:ALA:HB2   | 1:19:A:PHE:HD2   | 9        | 0.62          |
| (1,1595) | 1:16:A:ALA:HB2   | 1:19:A:PHE:HD2   | 16       | 0.62          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 1        | 0.62          |
| (1,1591) | 1:105:A:VAL:HG11 | 1:107:A:SER:HB2  | 14       | 0.62          |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD12  | 3        | 0.62          |
| (1,1514) | 1:18:A:LEU:HD22  | 1:13:A:ILE:HA    | 13       | 0.62          |
| (1,1341) | 1:29:A:LEU:HD11  | 1:147:A:VAL:HA   | 5        | 0.62          |
| (1,1340) | 1:128:A:ILE:HD11 | 1:98:A:ILE:HG23  | 3        | 0.62          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 16       | 0.62          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD13 | 4        | 0.62          |
| (1,1038) | 1:18:A:LEU:HA    | 1:18:A:LEU:HD23  | 12       | 0.62          |
| (1,955)  | 1:11:A:THR:HG21  | 1:9:A:THR:HA     | 13       | 0.62          |
| (1,884)  | 1:2:A:VAL:HG23   | 1:119:A:LYS:HG3  | 17       | 0.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 4        | 0.62          |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 15       | 0.62          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG22  | 15       | 0.62          |
| (1,581)  | 1:105:A:VAL:H    | 1:103:A:LYS:HG2  | 10       | 0.62          |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 4        | 0.62          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 16       | 0.62          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 16       | 0.62          |
| (3,154)  | 1:85:A:LEU:HD22  | 1:83:A:CYS:HB3   | 18       | 0.61          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 1        | 0.61          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 2        | 0.61          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 4        | 0.61          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 6        | 0.61          |
| (1,1697) | 1:151:A:LEU:HD13 | 1:150:A:TYR:HD2  | 8        | 0.61          |
| (1,1694) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HA   | 11       | 0.61          |
| (1,1682) | 1:149:A:ALA:HA   | 1:152:A:LEU:HD21 | 12       | 0.61          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 2        | 0.61          |
| (1,1595) | 1:16:A:ALA:HB2   | 1:19:A:PHE:HD1   | 17       | 0.61          |
| (1,1556) | 1:104:A:LEU:HD11 | 1:79:A:PHE:HB3   | 11       | 0.61          |
| (1,1450) | 1:71:A:ILE:HG22  | 1:70:A:ARG:HE    | 2        | 0.61          |
| (1,1450) | 1:71:A:ILE:HG22  | 1:70:A:ARG:HE    | 4        | 0.61          |
| (1,1308) | 1:71:A:ILE:HD12  | 1:83:A:CYS:HB3   | 5        | 0.61          |
| (1,1308) | 1:71:A:ILE:HD12  | 1:83:A:CYS:HB3   | 13       | 0.61          |
| (1,1304) | 1:56:A:ILE:HD11  | 1:27:A:ASP:HA    | 2        | 0.61          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 11       | 0.61          |
| (1,1023) | 1:17:A:ARG:HA    | 1:20:A:LYS:HE3   | 11       | 0.61          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 6        | 0.61          |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 13       | 0.61          |
| (1,811)  | 1:148:A:GLU:H    | 1:151:A:LEU:HB3  | 13       | 0.61          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD13  | 6        | 0.61          |
| (1,375)  | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 4        | 0.61          |
| (3,179)  | 1:148:A:GLU:HA   | 1:18:A:LEU:HD22  | 14       | 0.6           |
| (3,154)  | 1:85:A:LEU:HD23  | 1:83:A:CYS:HB3   | 10       | 0.6           |
| (1,1764) | 1:122:A:THR:HB   | 1:126:A:HIS:HB2  | 20       | 0.6           |
| (1,1701) | 1:153:A:ALA:HB3  | 1:154:A:ASN:HD22 | 3        | 0.6           |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 9        | 0.6           |
| (1,1574) | 1:128:A:ILE:HD13 | 1:91:A:ILE:HD13  | 7        | 0.6           |
| (1,1543) | 1:156:A:ALA:HB3  | 1:154:A:ASN:HA   | 1        | 0.6           |
| (1,1541) | 1:143:A:ILE:HA   | 1:30:A:ILE:HG12  | 18       | 0.6           |
| (1,1514) | 1:18:A:LEU:HD21  | 1:13:A:ILE:HA    | 11       | 0.6           |
| (1,1308) | 1:71:A:ILE:HD11  | 1:83:A:CYS:HB3   | 14       | 0.6           |
| (1,1243) | 1:53:A:ILE:HG12  | 1:45:A:GLU:HG3   | 16       | 0.6           |
| (1,1204) | 1:38:A:ILE:HD13  | 1:58:A:PHE:HZ    | 3        | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1204) | 1:38:A:ILE:HD13  | 1:58:A:PHE:HZ    | 4        | 0.6           |
| (1,1146) | 1:31:A:PRO:HG2   | 1:41:A:SER:HB2   | 1        | 0.6           |
| (1,1141) | 1:102:A:ILE:HG21 | 1:116:A:SER:HB3  | 9        | 0.6           |
| (1,1127) | 1:71:A:ILE:HG23  | 1:82:A:ALA:HA    | 9        | 0.6           |
| (1,955)  | 1:11:A:THR:HG23  | 1:9:A:THR:HA     | 20       | 0.6           |
| (1,875)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:H    | 1        | 0.6           |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 2        | 0.6           |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 16       | 0.6           |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 19       | 0.6           |
| (1,764)  | 1:139:A:GLU:H    | 1:139:A:GLU:HB2  | 4        | 0.6           |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD21  | 5        | 0.6           |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 5        | 0.6           |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 12       | 0.6           |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 5        | 0.6           |
| (1,375)  | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 9        | 0.6           |
| (1,233)  | 1:70:A:ARG:HH22  | 1:70:A:ARG:HB2   | 3        | 0.6           |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB3   | 20       | 0.6           |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 7        | 0.6           |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 13       | 0.59          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 14       | 0.59          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HG3   | 15       | 0.59          |
| (1,1697) | 1:151:A:LEU:HD13 | 1:150:A:TYR:HD1  | 19       | 0.59          |
| (1,1682) | 1:149:A:ALA:HA   | 1:152:A:LEU:HD21 | 20       | 0.59          |
| (1,1595) | 1:16:A:ALA:HB1   | 1:19:A:PHE:HD1   | 4        | 0.59          |
| (1,1595) | 1:16:A:ALA:HB2   | 1:19:A:PHE:HD2   | 7        | 0.59          |
| (1,1595) | 1:16:A:ALA:HB1   | 1:19:A:PHE:HD1   | 8        | 0.59          |
| (1,1595) | 1:16:A:ALA:HB2   | 1:19:A:PHE:HD1   | 11       | 0.59          |
| (1,1595) | 1:16:A:ALA:HB3   | 1:19:A:PHE:HD2   | 20       | 0.59          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 5        | 0.59          |
| (1,1557) | 1:85:A:LEU:HD11  | 1:91:A:ILE:HG12  | 5        | 0.59          |
| (1,1557) | 1:85:A:LEU:HD13  | 1:91:A:ILE:HG12  | 7        | 0.59          |
| (1,1556) | 1:104:A:LEU:HD11 | 1:79:A:PHE:HB3   | 8        | 0.59          |
| (1,1543) | 1:156:A:ALA:HB2  | 1:154:A:ASN:HA   | 2        | 0.59          |
| (1,1383) | 1:130:A:GLU:HG2  | 1:133:A:ILE:HG12 | 12       | 0.59          |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD12  | 19       | 0.59          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD11 | 7        | 0.59          |
| (1,955)  | 1:11:A:THR:HG21  | 1:9:A:THR:HA     | 15       | 0.59          |
| (1,884)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HG3  | 6        | 0.59          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 1        | 0.59          |
| (1,764)  | 1:139:A:GLU:H    | 1:139:A:GLU:HB2  | 19       | 0.59          |
| (1,764)  | 1:139:A:GLU:H    | 1:139:A:GLU:HB2  | 20       | 0.59          |
| (1,720)  | 1:128:A:ILE:H    | 1:128:A:ILE:HG13 | 15       | 0.59          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 8        | 0.59          |
| (1,565)  | 1:104:A:LEU:H    | 1:103:A:LYS:HG2  | 14       | 0.59          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD23  | 1        | 0.59          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 1        | 0.59          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD11  | 10       | 0.59          |
| (1,365)  | 1:67:A:VAL:H     | 1:67:A:VAL:HG13  | 11       | 0.59          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 4        | 0.59          |
| (1,162)  | 1:24:A:LEU:H     | 1:20:A:LYS:HB3   | 14       | 0.59          |
| (3,179)  | 1:148:A:GLU:HA   | 1:18:A:LEU:HD23  | 19       | 0.58          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 6        | 0.58          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 17       | 0.58          |
| (1,1764) | 1:122:A:THR:HB   | 1:126:A:HIS:HB2  | 2        | 0.58          |
| (1,1697) | 1:151:A:LEU:HD13 | 1:150:A:TYR:HD2  | 17       | 0.58          |
| (1,1697) | 1:151:A:LEU:HD13 | 1:150:A:TYR:HD2  | 18       | 0.58          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 5        | 0.58          |
| (1,1574) | 1:128:A:ILE:HD12 | 1:91:A:ILE:HD11  | 14       | 0.58          |
| (1,1555) | 1:104:A:LEU:HD11 | 1:114:A:LEU:HA   | 2        | 0.58          |
| (1,1429) | 1:104:A:LEU:HD13 | 1:106:A:ALA:H    | 16       | 0.58          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 2        | 0.58          |
| (1,955)  | 1:11:A:THR:HG23  | 1:9:A:THR:HA     | 14       | 0.58          |
| (1,955)  | 1:11:A:THR:HG22  | 1:9:A:THR:HA     | 17       | 0.58          |
| (1,885)  | 1:2:A:VAL:HG21   | 1:4:A:THR:HG23   | 3        | 0.58          |
| (1,849)  | 1:17:A:ARG:HH11  | 1:155:A:PRO:HG3  | 11       | 0.58          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG22  | 17       | 0.58          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD12  | 18       | 0.58          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 10       | 0.58          |
| (1,565)  | 1:104:A:LEU:H    | 1:103:A:LYS:HG2  | 15       | 0.58          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 7        | 0.58          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD11  | 7        | 0.58          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD11  | 19       | 0.58          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 12       | 0.58          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 15       | 0.58          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 6        | 0.58          |
| (1,265)  | 1:46:A:GLY:H     | 1:43:A:ILE:HG23  | 3        | 0.58          |
| (1,239)  | 1:42:A:GLU:H     | 1:55:A:LYS:HG2   | 10       | 0.58          |
| (3,154)  | 1:85:A:LEU:HD21  | 1:83:A:CYS:HB3   | 3        | 0.57          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE2   | 1        | 0.57          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 5        | 0.57          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 7        | 0.57          |
| (1,1701) | 1:153:A:ALA:HB2  | 1:154:A:ASN:HD22 | 8        | 0.57          |
| (1,1697) | 1:151:A:LEU:HD11 | 1:150:A:TYR:HD1  | 4        | 0.57          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 13       | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1450) | 1:71:A:ILE:HG23  | 1:70:A:ARG:HE    | 1        | 0.57          |
| (1,1038) | 1:18:A:LEU:HA    | 1:18:A:LEU:HD23  | 9        | 0.57          |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3  | 8        | 0.57          |
| (1,777)  | 1:142:A:GLY:H    | 1:141:A:SER:HB3  | 20       | 0.57          |
| (1,764)  | 1:139:A:GLU:H    | 1:139:A:GLU:HB2  | 2        | 0.57          |
| (1,764)  | 1:139:A:GLU:H    | 1:139:A:GLU:HB2  | 11       | 0.57          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB1  | 5        | 0.57          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB1  | 17       | 0.57          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 3        | 0.57          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 1        | 0.57          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB2   | 5        | 0.57          |
| (3,179)  | 1:148:A:GLU:HA   | 1:18:A:LEU:HD22  | 6        | 0.56          |
| (1,1764) | 1:122:A:THR:HB   | 1:126:A:HIS:HB2  | 19       | 0.56          |
| (1,1696) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HB   | 9        | 0.56          |
| (1,1694) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HA   | 1        | 0.56          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 12       | 0.56          |
| (1,1595) | 1:16:A:ALA:HB3   | 1:19:A:PHE:HD2   | 3        | 0.56          |
| (1,1557) | 1:85:A:LEU:HD11  | 1:91:A:ILE:HG12  | 2        | 0.56          |
| (1,1556) | 1:104:A:LEU:HD11 | 1:79:A:PHE:HB3   | 13       | 0.56          |
| (1,1450) | 1:71:A:ILE:HG21  | 1:70:A:ARG:HE    | 9        | 0.56          |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD12  | 14       | 0.56          |
| (1,1340) | 1:128:A:ILE:HD13 | 1:98:A:ILE:HG23  | 2        | 0.56          |
| (1,1304) | 1:56:A:ILE:HD11  | 1:27:A:ASP:HA    | 4        | 0.56          |
| (1,1259) | 1:8:A:GLU:HG3    | 1:114:A:LEU:H    | 4        | 0.56          |
| (1,1204) | 1:38:A:ILE:HD11  | 1:58:A:PHE:HZ    | 6        | 0.56          |
| (1,1127) | 1:71:A:ILE:HG21  | 1:82:A:ALA:HA    | 10       | 0.56          |
| (1,1127) | 1:71:A:ILE:HG22  | 1:82:A:ALA:HA    | 15       | 0.56          |
| (1,1038) | 1:18:A:LEU:HA    | 1:18:A:LEU:HD23  | 8        | 0.56          |
| (1,885)  | 1:2:A:VAL:HG23   | 1:4:A:THR:HG21   | 20       | 0.56          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 12       | 0.56          |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3  | 15       | 0.56          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 8        | 0.56          |
| (1,764)  | 1:139:A:GLU:H    | 1:139:A:GLU:HB2  | 14       | 0.56          |
| (1,720)  | 1:128:A:ILE:H    | 1:128:A:ILE:HG13 | 20       | 0.56          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 5        | 0.56          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 11       | 0.56          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD11  | 13       | 0.56          |
| (1,216)  | 1:38:A:ILE:H     | 1:38:A:ILE:HG13  | 3        | 0.56          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB2   | 11       | 0.56          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB1   | 15       | 0.56          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 13       | 0.56          |
| (3,58)   | 1:121:A:HIS:H    | 1:91:A:ILE:HD12  | 9        | 0.55          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1623) | 1:117:A:THR:HB   | 1:101:A:GLU:HB3 | 8        | 0.55          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2  | 17       | 0.55          |
| (1,1543) | 1:156:A:ALA:HB3  | 1:154:A:ASN:HA  | 18       | 0.55          |
| (1,1543) | 1:156:A:ALA:HB1  | 1:154:A:ASN:HA  | 19       | 0.55          |
| (1,1450) | 1:71:A:ILE:HG21  | 1:70:A:ARG:HE   | 19       | 0.55          |
| (1,1304) | 1:56:A:ILE:HD13  | 1:27:A:ASP:HA   | 12       | 0.55          |
| (1,1271) | 1:48:A:GLY:HA2   | 1:71:A:ILE:HG12 | 18       | 0.55          |
| (1,1166) | 1:33:A:VAL:HG13  | 1:29:A:LEU:H    | 9        | 0.55          |
| (1,1146) | 1:31:A:PRO:HG2   | 1:41:A:SER:HB2  | 9        | 0.55          |
| (1,1133) | 1:91:A:ILE:HG21  | 1:95:A:LEU:HB3  | 12       | 0.55          |
| (1,1127) | 1:71:A:ILE:HG21  | 1:82:A:ALA:HA   | 14       | 0.55          |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD12 | 5        | 0.55          |
| (1,1018) | 1:16:A:ALA:HB1   | 1:17:A:ARG:HA   | 6        | 0.55          |
| (1,1018) | 1:16:A:ALA:HB2   | 1:17:A:ARG:HA   | 15       | 0.55          |
| (1,955)  | 1:11:A:THR:HG22  | 1:9:A:THR:HA    | 3        | 0.55          |
| (1,955)  | 1:11:A:THR:HG21  | 1:9:A:THR:HA    | 11       | 0.55          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA  | 8        | 0.55          |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3 | 11       | 0.55          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11 | 8        | 0.55          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB2 | 3        | 0.55          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG23 | 10       | 0.55          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD13 | 5        | 0.55          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD11 | 10       | 0.55          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3 | 14       | 0.55          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2 | 2        | 0.55          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2 | 16       | 0.55          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2 | 17       | 0.55          |
| (1,565)  | 1:104:A:LEU:H    | 1:103:A:LYS:HG2 | 1        | 0.55          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD12 | 3        | 0.55          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD13 | 8        | 0.55          |
| (1,479)  | 1:87:A:GLU:H     | 1:68:A:LYS:HB3  | 11       | 0.55          |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3  | 18       | 0.55          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB3  | 1        | 0.55          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB3  | 3        | 0.55          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB1  | 1        | 0.54          |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD12 | 2        | 0.54          |
| (1,1556) | 1:104:A:LEU:HD13 | 1:79:A:PHE:HB3  | 9        | 0.54          |
| (1,1556) | 1:104:A:LEU:HD13 | 1:79:A:PHE:HB3  | 18       | 0.54          |
| (1,1543) | 1:156:A:ALA:HB2  | 1:154:A:ASN:HA  | 3        | 0.54          |
| (1,1543) | 1:156:A:ALA:HB2  | 1:154:A:ASN:HA  | 15       | 0.54          |
| (1,1436) | 1:91:A:ILE:HA    | 1:91:A:ILE:HD12 | 16       | 0.54          |
| (1,1300) | 1:71:A:ILE:HD13  | 1:70:A:ARG:HE   | 11       | 0.54          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 6        | 0.54          |
| (1,1247) | 1:102:A:ILE:HG21 | 1:81:A:TYR:HB3   | 20       | 0.54          |
| (1,1232) | 1:133:A:ILE:HG13 | 1:132:A:GLN:HB2  | 12       | 0.54          |
| (1,1204) | 1:38:A:ILE:HD11  | 1:58:A:PHE:HZ    | 9        | 0.54          |
| (1,1133) | 1:91:A:ILE:HG23  | 1:95:A:LEU:HB3   | 1        | 0.54          |
| (1,1038) | 1:18:A:LEU:HA    | 1:18:A:LEU:HD23  | 18       | 0.54          |
| (1,1030) | 1:55:A:LYS:HE3   | 1:44:A:ILE:HD12  | 18       | 0.54          |
| (1,1018) | 1:16:A:ALA:HB1   | 1:17:A:ARG:HA    | 3        | 0.54          |
| (1,1018) | 1:16:A:ALA:HB3   | 1:17:A:ARG:HA    | 10       | 0.54          |
| (1,1018) | 1:16:A:ALA:HB1   | 1:17:A:ARG:HA    | 12       | 0.54          |
| (1,955)  | 1:11:A:THR:HG23  | 1:9:A:THR:HA     | 7        | 0.54          |
| (1,955)  | 1:11:A:THR:HG23  | 1:9:A:THR:HA     | 10       | 0.54          |
| (1,955)  | 1:11:A:THR:HG23  | 1:9:A:THR:HA     | 16       | 0.54          |
| (1,885)  | 1:2:A:VAL:HG22   | 1:4:A:THR:HG23   | 13       | 0.54          |
| (1,875)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:H    | 5        | 0.54          |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3  | 18       | 0.54          |
| (1,777)  | 1:142:A:GLY:H    | 1:141:A:SER:HB3  | 3        | 0.54          |
| (1,764)  | 1:139:A:GLU:H    | 1:139:A:GLU:HB2  | 15       | 0.54          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB1  | 2        | 0.54          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB1  | 16       | 0.54          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG21  | 18       | 0.54          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 5        | 0.54          |
| (1,565)  | 1:104:A:LEU:H    | 1:103:A:LYS:HG2  | 20       | 0.54          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD12  | 18       | 0.54          |
| (1,300)  | 1:53:A:ILE:H     | 1:71:A:ILE:HG13  | 10       | 0.54          |
| (1,254)  | 1:45:A:GLU:H     | 1:53:A:ILE:HG12  | 16       | 0.54          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB1   | 4        | 0.54          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB1   | 14       | 0.54          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB2   | 17       | 0.54          |
| (3,121)  | 1:102:A:ILE:HD11 | 1:100:A:TYR:HB2  | 9        | 0.53          |
| (1,1701) | 1:153:A:ALA:HB1  | 1:154:A:ASN:HD22 | 18       | 0.53          |
| (1,1682) | 1:149:A:ALA:HA   | 1:152:A:LEU:HD23 | 14       | 0.53          |
| (1,1623) | 1:117:A:THR:HB   | 1:101:A:GLU:HB3  | 7        | 0.53          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 15       | 0.53          |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD12  | 1        | 0.53          |
| (1,1436) | 1:91:A:ILE:HA    | 1:91:A:ILE:HD11  | 11       | 0.53          |
| (1,1336) | 1:128:A:ILE:HD11 | 1:120:A:TYR:HB2  | 12       | 0.53          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 1        | 0.53          |
| (1,1166) | 1:33:A:VAL:HG12  | 1:29:A:LEU:H     | 6        | 0.53          |
| (1,1166) | 1:33:A:VAL:HG13  | 1:29:A:LEU:H     | 7        | 0.53          |
| (1,1032) | 1:20:A:LYS:HE2   | 1:20:A:LYS:HB2   | 15       | 0.53          |
| (1,1018) | 1:16:A:ALA:HB3   | 1:17:A:ARG:HA    | 11       | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1018) | 1:16:A:ALA:HB2   | 1:17:A:ARG:HA    | 18       | 0.53          |
| (1,1018) | 1:16:A:ALA:HB1   | 1:17:A:ARG:HA    | 19       | 0.53          |
| (1,777)  | 1:142:A:GLY:H    | 1:141:A:SER:HB3  | 19       | 0.53          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 6        | 0.53          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 12       | 0.53          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 8        | 0.53          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 15       | 0.53          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD13  | 2        | 0.53          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD13  | 9        | 0.53          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 8        | 0.53          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB2   | 7        | 0.53          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB1   | 8        | 0.53          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB2   | 9        | 0.53          |
| (3,108)  | 1:151:A:LEU:HA   | 1:17:A:ARG:HD3   | 18       | 0.52          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 19       | 0.52          |
| (1,1624) | 1:118:A:SER:HB2  | 1:119:A:LYS:HB2  | 14       | 0.52          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 5        | 0.52          |
| (1,1571) | 1:128:A:ILE:HD13 | 1:120:A:TYR:HA   | 14       | 0.52          |
| (1,1383) | 1:130:A:GLU:HG2  | 1:133:A:ILE:HG12 | 16       | 0.52          |
| (1,1204) | 1:38:A:ILE:HD12  | 1:58:A:PHE:HZ    | 11       | 0.52          |
| (1,1166) | 1:33:A:VAL:HG11  | 1:29:A:LEU:H     | 3        | 0.52          |
| (1,1133) | 1:91:A:ILE:HG21  | 1:95:A:LEU:HB3   | 2        | 0.52          |
| (1,1133) | 1:91:A:ILE:HG23  | 1:95:A:LEU:HB3   | 10       | 0.52          |
| (1,1018) | 1:16:A:ALA:HB1   | 1:17:A:ARG:HA    | 1        | 0.52          |
| (1,1018) | 1:16:A:ALA:HB2   | 1:17:A:ARG:HA    | 4        | 0.52          |
| (1,1018) | 1:16:A:ALA:HB3   | 1:17:A:ARG:HA    | 5        | 0.52          |
| (1,1018) | 1:16:A:ALA:HB2   | 1:17:A:ARG:HA    | 13       | 0.52          |
| (1,1018) | 1:16:A:ALA:HB2   | 1:17:A:ARG:HA    | 14       | 0.52          |
| (1,1018) | 1:16:A:ALA:HB1   | 1:17:A:ARG:HA    | 20       | 0.52          |
| (1,859)  | 1:78:A:ASN:HD21  | 1:77:A:ALA:HB2   | 10       | 0.52          |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD22 | 10       | 0.52          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 2        | 0.52          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB3  | 13       | 0.52          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB2  | 15       | 0.52          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG22  | 16       | 0.52          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 7        | 0.52          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 1        | 0.52          |
| (1,565)  | 1:104:A:LEU:H    | 1:103:A:LYS:HG2  | 9        | 0.52          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD11  | 17       | 0.52          |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 4        | 0.52          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 10       | 0.52          |
| (3,151)  | 1:104:A:LEU:HD21 | 1:18:A:LEU:HB3   | 12       | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,121)  | 1:102:A:ILE:HD11 | 1:100:A:TYR:HB2  | 10       | 0.51          |
| (3,58)   | 1:121:A:HIS:H    | 1:128:A:ILE:HG12 | 4        | 0.51          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE2   | 13       | 0.51          |
| (1,1661) | 1:143:A:ILE:HA   | 1:37:A:ALA:HB2   | 20       | 0.51          |
| (1,1574) | 1:128:A:ILE:HD12 | 1:91:A:ILE:HD12  | 18       | 0.51          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 14       | 0.51          |
| (1,1546) | 1:153:A:ALA:HB1  | 1:152:A:LEU:HA   | 16       | 0.51          |
| (1,1546) | 1:153:A:ALA:HB3  | 1:152:A:LEU:HA   | 19       | 0.51          |
| (1,1436) | 1:91:A:ILE:HA    | 1:91:A:ILE:HD13  | 6        | 0.51          |
| (1,1335) | 1:128:A:ILE:HD12 | 1:128:A:ILE:HA   | 1        | 0.51          |
| (1,1246) | 1:102:A:ILE:HG23 | 1:81:A:TYR:HB2   | 1        | 0.51          |
| (1,1223) | 1:8:A:GLU:HG2    | 1:113:A:ILE:HG23 | 2        | 0.51          |
| (1,1204) | 1:38:A:ILE:HD11  | 1:58:A:PHE:HZ    | 8        | 0.51          |
| (1,1204) | 1:38:A:ILE:HD11  | 1:58:A:PHE:HZ    | 14       | 0.51          |
| (1,1127) | 1:71:A:ILE:HG23  | 1:82:A:ALA:HA    | 3        | 0.51          |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD11  | 9        | 0.51          |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD12  | 18       | 0.51          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD12 | 14       | 0.51          |
| (1,1038) | 1:18:A:LEU:HA    | 1:18:A:LEU:HD23  | 3        | 0.51          |
| (1,1018) | 1:16:A:ALA:HB3   | 1:17:A:ARG:HA    | 2        | 0.51          |
| (1,1018) | 1:16:A:ALA:HB3   | 1:17:A:ARG:HA    | 9        | 0.51          |
| (1,955)  | 1:11:A:THR:HG21  | 1:9:A:THR:HA     | 5        | 0.51          |
| (1,955)  | 1:11:A:THR:HG22  | 1:9:A:THR:HA     | 9        | 0.51          |
| (1,955)  | 1:11:A:THR:HG22  | 1:9:A:THR:HA     | 19       | 0.51          |
| (1,929)  | 1:9:A:THR:HG23   | 1:22:A:PHE:HD2   | 1        | 0.51          |
| (1,929)  | 1:9:A:THR:HG23   | 1:22:A:PHE:HD2   | 2        | 0.51          |
| (1,884)  | 1:2:A:VAL:HG23   | 1:119:A:LYS:HG3  | 4        | 0.51          |
| (1,849)  | 1:17:A:ARG:HH11  | 1:155:A:PRO:HG3  | 14       | 0.51          |
| (1,828)  | 1:153:A:ALA:H    | 1:149:A:ALA:HB3  | 19       | 0.51          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB1  | 9        | 0.51          |
| (1,720)  | 1:128:A:ILE:H    | 1:128:A:ILE:HG13 | 2        | 0.51          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD11  | 20       | 0.51          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 8        | 0.51          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 20       | 0.51          |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG13 | 17       | 0.51          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 18       | 0.51          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 12       | 0.51          |
| (1,584)  | 1:106:A:ALA:H    | 1:105:A:VAL:HG11 | 12       | 0.51          |
| (1,535)  | 1:100:A:TYR:H    | 1:83:A:CYS:HB3   | 19       | 0.51          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 18       | 0.51          |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 6        | 0.51          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB3   | 6        | 0.51          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB3  | 19       | 0.51          |
| (3,167)  | 1:146:A:ALA:HB2  | 1:35:A:PRO:HD3  | 16       | 0.5           |
| (3,151)  | 1:104:A:LEU:HD23 | 1:114:A:LEU:HG  | 8        | 0.5           |
| (1,1703) | 1:154:A:ASN:HB3  | 1:17:A:ARG:HH11 | 1        | 0.5           |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB2  | 2        | 0.5           |
| (1,1623) | 1:117:A:THR:HB   | 1:101:A:GLU:HB3 | 5        | 0.5           |
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG23 | 18       | 0.5           |
| (1,1546) | 1:153:A:ALA:HB1  | 1:152:A:LEU:HA  | 2        | 0.5           |
| (1,1546) | 1:153:A:ALA:HB2  | 1:152:A:LEU:HA  | 13       | 0.5           |
| (1,1543) | 1:156:A:ALA:HB1  | 1:154:A:ASN:HA  | 5        | 0.5           |
| (1,1514) | 1:18:A:LEU:HD22  | 1:13:A:ILE:HA   | 10       | 0.5           |
| (1,1446) | 1:56:A:ILE:HD13  | 1:40:A:SER:HA   | 12       | 0.5           |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD12 | 9        | 0.5           |
| (1,1341) | 1:29:A:LEU:HD12  | 1:147:A:VAL:HA  | 3        | 0.5           |
| (1,1328) | 1:104:A:LEU:HD12 | 1:112:A:SER:HB3 | 17       | 0.5           |
| (1,1289) | 1:52:A:THR:HB    | 1:71:A:ILE:HG22 | 17       | 0.5           |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG22 | 18       | 0.5           |
| (1,1230) | 1:98:A:ILE:HG23  | 1:85:A:LEU:HG   | 7        | 0.5           |
| (1,1204) | 1:38:A:ILE:HD12  | 1:58:A:PHE:HZ   | 10       | 0.5           |
| (1,1166) | 1:33:A:VAL:HG11  | 1:29:A:LEU:H    | 5        | 0.5           |
| (1,1153) | 1:132:A:GLN:HA   | 1:132:A:GLN:HG2 | 7        | 0.5           |
| (1,1141) | 1:102:A:ILE:HG21 | 1:116:A:SER:HB3 | 2        | 0.5           |
| (1,1120) | 1:74:A:ILE:HD11  | 1:71:A:ILE:HA   | 12       | 0.5           |
| (1,1043) | 1:18:A:LEU:HD23  | 1:22:A:PHE:HD1  | 16       | 0.5           |
| (1,1018) | 1:16:A:ALA:HB3   | 1:17:A:ARG:HA   | 17       | 0.5           |
| (1,955)  | 1:11:A:THR:HG23  | 1:9:A:THR:HA    | 18       | 0.5           |
| (1,929)  | 1:9:A:THR:HG21   | 1:22:A:PHE:HD2  | 13       | 0.5           |
| (1,929)  | 1:9:A:THR:HG21   | 1:22:A:PHE:HD2  | 20       | 0.5           |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA  | 13       | 0.5           |
| (1,849)  | 1:17:A:ARG:HH11  | 1:155:A:PRO:HG3 | 9        | 0.5           |
| (1,847)  | 1:17:A:ARG:HH11  | 1:151:A:LEU:HA  | 10       | 0.5           |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3 | 20       | 0.5           |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3 | 20       | 0.5           |
| (1,823)  | 1:153:A:ALA:H    | 1:17:A:ARG:HH11 | 17       | 0.5           |
| (1,777)  | 1:142:A:GLY:H    | 1:141:A:SER:HB3 | 2        | 0.5           |
| (1,777)  | 1:142:A:GLY:H    | 1:141:A:SER:HB3 | 7        | 0.5           |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB3 | 1        | 0.5           |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG21 | 3        | 0.5           |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG21 | 4        | 0.5           |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3 | 3        | 0.5           |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3 | 10       | 0.5           |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3 | 13       | 0.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 15       | 0.5           |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG11 | 3        | 0.5           |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 20       | 0.5           |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD11  | 16       | 0.5           |
| (1,163)  | 1:24:A:LEU:H     | 1:21:A:ALA:HB1   | 20       | 0.5           |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB2   | 2        | 0.5           |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB2   | 16       | 0.5           |
| (3,153)  | 1:113:A:ILE:HD11 | 1:108:A:PRO:HG2  | 15       | 0.49          |
| (3,51)   | 1:114:A:LEU:H    | 1:8:A:GLU:HB3    | 8        | 0.49          |
| (1,1694) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HA   | 15       | 0.49          |
| (1,1694) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HA   | 16       | 0.49          |
| (1,1661) | 1:143:A:ILE:HA   | 1:37:A:ALA:HB2   | 10       | 0.49          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB3   | 4        | 0.49          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB2   | 6        | 0.49          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB1   | 12       | 0.49          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB1   | 18       | 0.49          |
| (1,1571) | 1:128:A:ILE:HD11 | 1:120:A:TYR:HA   | 12       | 0.49          |
| (1,1304) | 1:56:A:ILE:HD13  | 1:27:A:ASP:HA    | 10       | 0.49          |
| (1,1238) | 1:43:A:ILE:HD13  | 1:48:A:GLY:HA2   | 10       | 0.49          |
| (1,1238) | 1:43:A:ILE:HD11  | 1:48:A:GLY:HA2   | 15       | 0.49          |
| (1,1223) | 1:8:A:GLU:HG2    | 1:113:A:ILE:HG22 | 12       | 0.49          |
| (1,1204) | 1:38:A:ILE:HD12  | 1:58:A:PHE:HZ    | 17       | 0.49          |
| (1,1166) | 1:33:A:VAL:HG11  | 1:29:A:LEU:H     | 17       | 0.49          |
| (1,1127) | 1:71:A:ILE:HG23  | 1:82:A:ALA:HA    | 19       | 0.49          |
| (1,1120) | 1:74:A:ILE:HD11  | 1:71:A:ILE:HA    | 1        | 0.49          |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD13  | 16       | 0.49          |
| (1,1018) | 1:16:A:ALA:HB2   | 1:17:A:ARG:HA    | 8        | 0.49          |
| (1,929)  | 1:9:A:THR:HG21   | 1:22:A:PHE:HD2   | 8        | 0.49          |
| (1,929)  | 1:9:A:THR:HG23   | 1:22:A:PHE:HD2   | 12       | 0.49          |
| (1,905)  | 1:4:A:THR:HG21   | 1:119:A:LYS:HB2  | 6        | 0.49          |
| (1,885)  | 1:2:A:VAL:HG23   | 1:4:A:THR:HG23   | 15       | 0.49          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 10       | 0.49          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 14       | 0.49          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB2  | 7        | 0.49          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG21  | 2        | 0.49          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG23  | 20       | 0.49          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 1        | 0.49          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 2        | 0.49          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 18       | 0.49          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 12       | 0.49          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 2        | 0.49          |
| (1,565)  | 1:104:A:LEU:H    | 1:103:A:LYS:HG2  | 3        | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,233)  | 1:70:A:ARG:HH22  | 1:70:A:ARG:HB2   | 15       | 0.49          |
| (1,162)  | 1:24:A:LEU:H     | 1:20:A:LYS:HB3   | 9        | 0.49          |
| (1,23)   | 1:32:A:LYS:H     | 1:31:A:PRO:HB3   | 18       | 0.49          |
| (3,147)  | 1:80:A:THR:HA    | 1:103:A:LYS:HD2  | 6        | 0.48          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE1   | 7        | 0.48          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE1   | 9        | 0.48          |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG21  | 17       | 0.48          |
| (1,1697) | 1:151:A:LEU:HD12 | 1:150:A:TYR:HD2  | 15       | 0.48          |
| (1,1623) | 1:117:A:THR:HB   | 1:101:A:GLU:HB3  | 13       | 0.48          |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG23 | 18       | 0.48          |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD13  | 8        | 0.48          |
| (1,1429) | 1:104:A:LEU:HD13 | 1:106:A:ALA:H    | 4        | 0.48          |
| (1,1291) | 1:52:A:THR:HB    | 1:46:A:GLY:HA2   | 3        | 0.48          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG21  | 5        | 0.48          |
| (1,1204) | 1:38:A:ILE:HD11  | 1:58:A:PHE:HZ    | 13       | 0.48          |
| (1,1183) | 1:34:A:ALA:HB2   | 1:147:A:VAL:HG13 | 20       | 0.48          |
| (1,1166) | 1:33:A:VAL:HG13  | 1:29:A:LEU:H     | 2        | 0.48          |
| (1,1166) | 1:33:A:VAL:HG13  | 1:29:A:LEU:H     | 10       | 0.48          |
| (1,1166) | 1:33:A:VAL:HG11  | 1:29:A:LEU:H     | 16       | 0.48          |
| (1,1120) | 1:74:A:ILE:HD12  | 1:71:A:ILE:HA    | 2        | 0.48          |
| (1,1120) | 1:74:A:ILE:HD13  | 1:71:A:ILE:HA    | 9        | 0.48          |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD12  | 11       | 0.48          |
| (1,1018) | 1:16:A:ALA:HB3   | 1:17:A:ARG:HA    | 7        | 0.48          |
| (1,996)  | 1:82:A:ALA:HB2   | 1:73:A:GLU:HG3   | 20       | 0.48          |
| (1,955)  | 1:11:A:THR:HG21  | 1:9:A:THR:HA     | 4        | 0.48          |
| (1,955)  | 1:11:A:THR:HG22  | 1:9:A:THR:HA     | 6        | 0.48          |
| (1,955)  | 1:11:A:THR:HG21  | 1:9:A:THR:HA     | 12       | 0.48          |
| (1,890)  | 1:2:A:VAL:HG11   | 1:4:A:THR:HB     | 14       | 0.48          |
| (1,885)  | 1:2:A:VAL:HG22   | 1:4:A:THR:HG22   | 19       | 0.48          |
| (1,823)  | 1:153:A:ALA:H    | 1:17:A:ARG:HH11  | 7        | 0.48          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB1  | 4        | 0.48          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB3  | 6        | 0.48          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB1  | 20       | 0.48          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 4        | 0.48          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 17       | 0.48          |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG11 | 14       | 0.48          |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG11 | 15       | 0.48          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 10       | 0.48          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 19       | 0.48          |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 19       | 0.48          |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 1        | 0.48          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB1   | 13       | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB1   | 18       | 0.48          |
| (3,100)  | 1:8:A:GLU:HB2    | 1:113:A:ILE:HG23 | 18       | 0.47          |
| (1,1694) | 1:151:A:LEU:HD13 | 1:147:A:VAL:HA   | 18       | 0.47          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB1   | 13       | 0.47          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 1        | 0.47          |
| (1,1588) | 1:105:A:VAL:HG12 | 1:105:A:VAL:H    | 8        | 0.47          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 11       | 0.47          |
| (1,1336) | 1:128:A:ILE:HD13 | 1:120:A:TYR:HB2  | 14       | 0.47          |
| (1,1271) | 1:48:A:GLY:HA2   | 1:71:A:ILE:HG12  | 7        | 0.47          |
| (1,1238) | 1:43:A:ILE:HD12  | 1:48:A:GLY:HA2   | 1        | 0.47          |
| (1,1234) | 1:133:A:ILE:HG13 | 1:128:A:ILE:HG21 | 18       | 0.47          |
| (1,1168) | 1:33:A:VAL:HG13  | 1:150:A:TYR:HB3  | 16       | 0.47          |
| (1,1129) | 1:30:A:ILE:HG22  | 1:37:A:ALA:H     | 8        | 0.47          |
| (1,1120) | 1:74:A:ILE:HD12  | 1:71:A:ILE:HA    | 7        | 0.47          |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD13  | 12       | 0.47          |
| (1,1018) | 1:16:A:ALA:HB3   | 1:17:A:ARG:HA    | 16       | 0.47          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 12       | 0.47          |
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD1   | 3        | 0.47          |
| (1,929)  | 1:9:A:THR:HG23   | 1:22:A:PHE:HD1   | 16       | 0.47          |
| (1,890)  | 1:2:A:VAL:HG12   | 1:4:A:THR:HB     | 6        | 0.47          |
| (1,890)  | 1:2:A:VAL:HG11   | 1:4:A:THR:HB     | 19       | 0.47          |
| (1,882)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HE2  | 6        | 0.47          |
| (1,882)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HE2  | 11       | 0.47          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 17       | 0.47          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 19       | 0.47          |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3  | 12       | 0.47          |
| (1,823)  | 1:153:A:ALA:H    | 1:17:A:ARG:HH11  | 11       | 0.47          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 5        | 0.47          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 7        | 0.47          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 12       | 0.47          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 20       | 0.47          |
| (1,777)  | 1:142:A:GLY:H    | 1:141:A:SER:HB3  | 6        | 0.47          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG23  | 1        | 0.47          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG21  | 6        | 0.47          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD11  | 13       | 0.47          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 9        | 0.47          |
| (1,534)  | 1:100:A:TYR:H    | 1:84:A:THR:HG21  | 19       | 0.47          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD21  | 8        | 0.47          |
| (1,479)  | 1:87:A:GLU:H     | 1:68:A:LYS:HB3   | 14       | 0.47          |
| (1,374)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB2   | 20       | 0.47          |
| (1,216)  | 1:38:A:ILE:H     | 1:38:A:ILE:HG13  | 5        | 0.47          |
| (1,96)   | 1:146:A:ALA:H    | 1:145:A:LYS:HB2  | 9        | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,158)  | 1:118:A:SER:HB2  | 1:6:A:GLU:HG2    | 13       | 0.46          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE1   | 6        | 0.46          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE1   | 16       | 0.46          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 3        | 0.46          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 10       | 0.46          |
| (1,1682) | 1:149:A:ALA:HA   | 1:152:A:LEU:HD21 | 6        | 0.46          |
| (1,1588) | 1:105:A:VAL:HG13 | 1:105:A:VAL:H    | 16       | 0.46          |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD12  | 10       | 0.46          |
| (1,1556) | 1:104:A:LEU:HD13 | 1:79:A:PHE:HB3   | 5        | 0.46          |
| (1,1510) | 1:84:A:THR:HG21  | 1:69:A:HIS:HA    | 8        | 0.46          |
| (1,1446) | 1:56:A:ILE:HD11  | 1:40:A:SER:HA    | 8        | 0.46          |
| (1,1429) | 1:104:A:LEU:HD11 | 1:106:A:ALA:H    | 7        | 0.46          |
| (1,1261) | 1:13:A:ILE:HB    | 1:18:A:LEU:HD22  | 13       | 0.46          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG23  | 19       | 0.46          |
| (1,1204) | 1:38:A:ILE:HD13  | 1:58:A:PHE:HZ    | 18       | 0.46          |
| (1,1204) | 1:38:A:ILE:HD13  | 1:58:A:PHE:HZ    | 20       | 0.46          |
| (1,1203) | 1:38:A:ILE:HD13  | 1:38:A:ILE:HA    | 10       | 0.46          |
| (1,1146) | 1:31:A:PRO:HG2   | 1:41:A:SER:HB2   | 13       | 0.46          |
| (1,1133) | 1:91:A:ILE:HG21  | 1:95:A:LEU:HB3   | 15       | 0.46          |
| (1,1120) | 1:74:A:ILE:HD12  | 1:71:A:ILE:HA    | 13       | 0.46          |
| (1,1120) | 1:74:A:ILE:HD11  | 1:71:A:ILE:HA    | 16       | 0.46          |
| (1,929)  | 1:9:A:THR:HG22   | 1:22:A:PHE:HD2   | 15       | 0.46          |
| (1,890)  | 1:2:A:VAL:HG13   | 1:4:A:THR:HB     | 8        | 0.46          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 2        | 0.46          |
| (1,870)  | 1:145:A:LYS:H    | 1:144:A:PHE:HB2  | 18       | 0.46          |
| (1,823)  | 1:153:A:ALA:H    | 1:17:A:ARG:HH11  | 1        | 0.46          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB3  | 8        | 0.46          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB2  | 11       | 0.46          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG22  | 7        | 0.46          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG22  | 9        | 0.46          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 16       | 0.46          |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG13 | 16       | 0.46          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 17       | 0.46          |
| (1,565)  | 1:104:A:LEU:H    | 1:103:A:LYS:HG2  | 19       | 0.46          |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 3        | 0.46          |
| (1,476)  | 1:86:A:ILE:H     | 1:86:A:ILE:HG22  | 20       | 0.46          |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 10       | 0.46          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 11       | 0.46          |
| (3,58)   | 1:121:A:HIS:H    | 1:128:A:ILE:HG12 | 17       | 0.45          |
| (3,14)   | 1:24:A:LEU:H     | 1:71:A:ILE:HD12  | 6        | 0.45          |
| (1,1701) | 1:153:A:ALA:HB3  | 1:154:A:ASN:HD22 | 10       | 0.45          |
| (1,1694) | 1:151:A:LEU:HD13 | 1:147:A:VAL:HA   | 17       | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1660) | 1:143:A:ILE:HA   | 1:144:A:PHE:HD2  | 20       | 0.45          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB2   | 10       | 0.45          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB3   | 16       | 0.45          |
| (1,1588) | 1:105:A:VAL:HG11 | 1:105:A:VAL:H    | 11       | 0.45          |
| (1,1588) | 1:105:A:VAL:HG12 | 1:105:A:VAL:H    | 20       | 0.45          |
| (1,1574) | 1:128:A:ILE:HD12 | 1:91:A:ILE:HD12  | 5        | 0.45          |
| (1,1571) | 1:128:A:ILE:HD11 | 1:120:A:TYR:HA   | 7        | 0.45          |
| (1,1335) | 1:128:A:ILE:HD11 | 1:128:A:ILE:HA   | 13       | 0.45          |
| (1,1300) | 1:71:A:ILE:HD11  | 1:70:A:ARG:HE    | 1        | 0.45          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG21  | 13       | 0.45          |
| (1,1223) | 1:8:A:GLU:HG2    | 1:113:A:ILE:HG22 | 17       | 0.45          |
| (1,1221) | 1:8:A:GLU:HB3    | 1:115:A:LYS:HA   | 8        | 0.45          |
| (1,1203) | 1:38:A:ILE:HD11  | 1:38:A:ILE:HA    | 2        | 0.45          |
| (1,1203) | 1:38:A:ILE:HD12  | 1:38:A:ILE:HA    | 14       | 0.45          |
| (1,1168) | 1:33:A:VAL:HG12  | 1:150:A:TYR:HB3  | 1        | 0.45          |
| (1,1168) | 1:33:A:VAL:HG12  | 1:150:A:TYR:HB3  | 11       | 0.45          |
| (1,1168) | 1:33:A:VAL:HG12  | 1:150:A:TYR:HB3  | 14       | 0.45          |
| (1,1166) | 1:33:A:VAL:HG11  | 1:29:A:LEU:H     | 4        | 0.45          |
| (1,1166) | 1:33:A:VAL:HG12  | 1:29:A:LEU:H     | 13       | 0.45          |
| (1,1166) | 1:33:A:VAL:HG12  | 1:29:A:LEU:H     | 20       | 0.45          |
| (1,1127) | 1:71:A:ILE:HG22  | 1:82:A:ALA:HA    | 11       | 0.45          |
| (1,1120) | 1:74:A:ILE:HD11  | 1:71:A:ILE:HA    | 5        | 0.45          |
| (1,1091) | 1:27:A:ASP:HA    | 1:41:A:SER:HB2   | 13       | 0.45          |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD13  | 17       | 0.45          |
| (1,929)  | 1:9:A:THR:HG21   | 1:22:A:PHE:HD2   | 10       | 0.45          |
| (1,929)  | 1:9:A:THR:HG22   | 1:22:A:PHE:HD1   | 14       | 0.45          |
| (1,929)  | 1:9:A:THR:HG23   | 1:22:A:PHE:HD1   | 19       | 0.45          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 19       | 0.45          |
| (1,823)  | 1:153:A:ALA:H    | 1:17:A:ARG:HH11  | 18       | 0.45          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 3        | 0.45          |
| (1,737)  | 1:132:A:GLN:H    | 1:132:A:GLN:HG2  | 19       | 0.45          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD11  | 16       | 0.45          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 19       | 0.45          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 13       | 0.45          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 15       | 0.45          |
| (1,479)  | 1:87:A:GLU:H     | 1:68:A:LYS:HB3   | 16       | 0.45          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 18       | 0.45          |
| (3,179)  | 1:148:A:GLU:HA   | 1:152:A:LEU:HD22 | 7        | 0.44          |
| (3,135)  | 1:115:A:LYS:HD3  | 1:8:A:GLU:HA     | 14       | 0.44          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 3        | 0.44          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 13       | 0.44          |
| (1,1694) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HA   | 7        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1654) | 1:133:A:ILE:HG22 | 1:5:A:TYR:HB2    | 2        | 0.44          |
| (1,1588) | 1:105:A:VAL:HG11 | 1:105:A:VAL:H    | 3        | 0.44          |
| (1,1588) | 1:105:A:VAL:HG13 | 1:105:A:VAL:H    | 9        | 0.44          |
| (1,1588) | 1:105:A:VAL:HG13 | 1:105:A:VAL:H    | 17       | 0.44          |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG23 | 2        | 0.44          |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG21 | 14       | 0.44          |
| (1,1556) | 1:104:A:LEU:HD13 | 1:79:A:PHE:HB3   | 1        | 0.44          |
| (1,1514) | 1:18:A:LEU:HD23  | 1:13:A:ILE:HA    | 2        | 0.44          |
| (1,1510) | 1:84:A:THR:HG23  | 1:69:A:HIS:HA    | 2        | 0.44          |
| (1,1350) | 1:56:A:ILE:HG23  | 1:38:A:ILE:HG12  | 11       | 0.44          |
| (1,1238) | 1:43:A:ILE:HD12  | 1:48:A:GLY:HA2   | 7        | 0.44          |
| (1,1172) | 1:34:A:ALA:HA    | 1:37:A:ALA:HB2   | 20       | 0.44          |
| (1,1166) | 1:33:A:VAL:HG13  | 1:29:A:LEU:H     | 11       | 0.44          |
| (1,1120) | 1:74:A:ILE:HD12  | 1:71:A:ILE:HA    | 14       | 0.44          |
| (1,976)  | 1:13:A:ILE:HG23  | 1:17:A:ARG:HB2   | 2        | 0.44          |
| (1,929)  | 1:9:A:THR:HG23   | 1:22:A:PHE:HD1   | 4        | 0.44          |
| (1,890)  | 1:2:A:VAL:HG13   | 1:4:A:THR:HB     | 1        | 0.44          |
| (1,890)  | 1:2:A:VAL:HG13   | 1:4:A:THR:HB     | 9        | 0.44          |
| (1,875)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:H    | 20       | 0.44          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 15       | 0.44          |
| (1,777)  | 1:142:A:GLY:H    | 1:141:A:SER:HB3  | 15       | 0.44          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG22  | 13       | 0.44          |
| (1,698)  | 1:121:A:HIS:H    | 1:121:A:HIS:HB3  | 11       | 0.44          |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG12 | 2        | 0.44          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 20       | 0.44          |
| (1,565)  | 1:104:A:LEU:H    | 1:103:A:LYS:HG2  | 4        | 0.44          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 16       | 0.44          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD12  | 4        | 0.44          |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 12       | 0.44          |
| (1,344)  | 1:64:A:PHE:H     | 1:57:A:THR:HG22  | 6        | 0.44          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 11       | 0.44          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 19       | 0.44          |
| (1,96)   | 1:146:A:ALA:H    | 1:145:A:LYS:HB2  | 12       | 0.44          |
| (1,96)   | 1:146:A:ALA:H    | 1:145:A:LYS:HB2  | 14       | 0.44          |
| (1,58)   | 1:9:A:THR:H      | 1:8:A:GLU:HG3    | 4        | 0.44          |
| (1,1696) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HB   | 2        | 0.43          |
| (1,1588) | 1:105:A:VAL:HG11 | 1:105:A:VAL:H    | 7        | 0.43          |
| (1,1510) | 1:84:A:THR:HG22  | 1:69:A:HIS:HA    | 1        | 0.43          |
| (1,1510) | 1:84:A:THR:HG21  | 1:69:A:HIS:HA    | 19       | 0.43          |
| (1,1429) | 1:104:A:LEU:HD13 | 1:106:A:ALA:H    | 20       | 0.43          |
| (1,1300) | 1:71:A:ILE:HD11  | 1:70:A:ARG:HE    | 4        | 0.43          |
| (1,1223) | 1:8:A:GLU:HG2    | 1:113:A:ILE:HG23 | 15       | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1120) | 1:74:A:ILE:HD13  | 1:71:A:ILE:HA    | 18       | 0.43          |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD12  | 1        | 0.43          |
| (1,929)  | 1:9:A:THR:HG23   | 1:22:A:PHE:HD2   | 9        | 0.43          |
| (1,885)  | 1:2:A:VAL:HG23   | 1:4:A:THR:HG21   | 11       | 0.43          |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3  | 7        | 0.43          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB1  | 14       | 0.43          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG22  | 8        | 0.43          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG22  | 11       | 0.43          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD13  | 9        | 0.43          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD13  | 14       | 0.43          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD11  | 19       | 0.43          |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG13 | 4        | 0.43          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 8        | 0.43          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 12       | 0.43          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 13       | 0.43          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 16       | 0.43          |
| (1,96)   | 1:146:A:ALA:H    | 1:145:A:LYS:HB2  | 7        | 0.43          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2   | 4        | 0.42          |
| (3,147)  | 1:80:A:THR:HA    | 1:103:A:LYS:HD3  | 5        | 0.42          |
| (3,58)   | 1:121:A:HIS:H    | 1:128:A:ILE:HG12 | 15       | 0.42          |
| (3,7)    | 1:13:A:ILE:H     | 1:17:A:ARG:HB2   | 18       | 0.42          |
| (1,1696) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HB   | 12       | 0.42          |
| (1,1694) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HA   | 10       | 0.42          |
| (1,1675) | 1:147:A:VAL:HG21 | 1:22:A:PHE:HB2   | 20       | 0.42          |
| (1,1588) | 1:105:A:VAL:HG11 | 1:105:A:VAL:H    | 5        | 0.42          |
| (1,1588) | 1:105:A:VAL:HG11 | 1:105:A:VAL:H    | 10       | 0.42          |
| (1,1588) | 1:105:A:VAL:HG12 | 1:105:A:VAL:H    | 13       | 0.42          |
| (1,1588) | 1:105:A:VAL:HG11 | 1:105:A:VAL:H    | 14       | 0.42          |
| (1,1588) | 1:105:A:VAL:HG11 | 1:105:A:VAL:H    | 18       | 0.42          |
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG23  | 10       | 0.42          |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD11  | 19       | 0.42          |
| (1,1510) | 1:84:A:THR:HG21  | 1:69:A:HIS:HA    | 7        | 0.42          |
| (1,1271) | 1:48:A:GLY:HA2   | 1:71:A:ILE:HG12  | 17       | 0.42          |
| (1,1203) | 1:38:A:ILE:HD11  | 1:38:A:ILE:HA    | 18       | 0.42          |
| (1,1153) | 1:132:A:GLN:HA   | 1:132:A:GLN:HG2  | 19       | 0.42          |
| (1,1134) | 1:30:A:ILE:HG21  | 1:37:A:ALA:HB2   | 8        | 0.42          |
| (1,1133) | 1:91:A:ILE:HG23  | 1:95:A:LEU:HB3   | 5        | 0.42          |
| (1,1032) | 1:20:A:LYS:HE2   | 1:20:A:LYS:HB2   | 19       | 0.42          |
| (1,994)  | 1:82:A:ALA:HB2   | 1:71:A:ILE:HA    | 9        | 0.42          |
| (1,976)  | 1:13:A:ILE:HG23  | 1:17:A:ARG:HB2   | 13       | 0.42          |
| (1,943)  | 1:117:A:THR:HG23 | 1:101:A:GLU:HB3  | 1        | 0.42          |
| (1,890)  | 1:2:A:VAL:HG11   | 1:4:A:THR:HB     | 18       | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,777)  | 1:142:A:GLY:H    | 1:141:A:SER:HB3  | 1        | 0.42          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 18       | 0.42          |
| (1,216)  | 1:38:A:ILE:H     | 1:38:A:ILE:HG13  | 16       | 0.42          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 7        | 0.42          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 20       | 0.42          |
| (1,96)   | 1:146:A:ALA:H    | 1:145:A:LYS:HB2  | 2        | 0.42          |
| (1,58)   | 1:9:A:THR:H      | 1:8:A:GLU:HG3    | 6        | 0.42          |
| (3,157)  | 1:114:A:LEU:HD23 | 1:22:A:PHE:HD2   | 12       | 0.41          |
| (3,154)  | 1:85:A:LEU:HD22  | 1:83:A:CYS:HB3   | 19       | 0.41          |
| (3,151)  | 1:104:A:LEU:HD21 | 1:114:A:LEU:HG   | 9        | 0.41          |
| (1,1588) | 1:105:A:VAL:HG11 | 1:105:A:VAL:H    | 1        | 0.41          |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG22 | 9        | 0.41          |
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG23  | 15       | 0.41          |
| (1,1510) | 1:84:A:THR:HG21  | 1:69:A:HIS:HA    | 4        | 0.41          |
| (1,1510) | 1:84:A:THR:HG22  | 1:69:A:HIS:HA    | 17       | 0.41          |
| (1,1340) | 1:128:A:ILE:HD13 | 1:98:A:ILE:HG21  | 15       | 0.41          |
| (1,1289) | 1:52:A:THR:HB    | 1:71:A:ILE:HG21  | 11       | 0.41          |
| (1,1246) | 1:102:A:ILE:HG21 | 1:81:A:TYR:HB2   | 20       | 0.41          |
| (1,1203) | 1:38:A:ILE:HD12  | 1:38:A:ILE:HA    | 6        | 0.41          |
| (1,1203) | 1:38:A:ILE:HD12  | 1:38:A:ILE:HA    | 13       | 0.41          |
| (1,1120) | 1:74:A:ILE:HD11  | 1:71:A:ILE:HA    | 4        | 0.41          |
| (1,1043) | 1:18:A:LEU:HD23  | 1:22:A:PHE:HD2   | 18       | 0.41          |
| (1,994)  | 1:82:A:ALA:HB2   | 1:71:A:ILE:HA    | 3        | 0.41          |
| (1,929)  | 1:9:A:THR:HG21   | 1:22:A:PHE:HD1   | 6        | 0.41          |
| (1,929)  | 1:9:A:THR:HG22   | 1:22:A:PHE:HD2   | 7        | 0.41          |
| (1,929)  | 1:9:A:THR:HG23   | 1:22:A:PHE:HD2   | 18       | 0.41          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 3        | 0.41          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 16       | 0.41          |
| (1,812)  | 1:148:A:GLU:H    | 1:152:A:LEU:HD21 | 12       | 0.41          |
| (1,777)  | 1:142:A:GLY:H    | 1:141:A:SER:HB3  | 5        | 0.41          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB1  | 10       | 0.41          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 7        | 0.41          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 3        | 0.41          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD13  | 6        | 0.41          |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 4        | 0.41          |
| (1,375)  | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 10       | 0.41          |
| (3,58)   | 1:121:A:HIS:H    | 1:128:A:ILE:HG12 | 16       | 0.4           |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE2   | 17       | 0.4           |
| (1,1696) | 1:151:A:LEU:HD13 | 1:147:A:VAL:HB   | 8        | 0.4           |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 13       | 0.4           |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 15       | 0.4           |
| (1,1588) | 1:105:A:VAL:HG13 | 1:105:A:VAL:H    | 19       | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG22  | 12       | 0.4           |
| (1,1510) | 1:84:A:THR:HG23  | 1:69:A:HIS:HA    | 11       | 0.4           |
| (1,1510) | 1:84:A:THR:HG23  | 1:69:A:HIS:HA    | 15       | 0.4           |
| (1,1146) | 1:31:A:PRO:HG2   | 1:41:A:SER:HB2   | 10       | 0.4           |
| (1,1111) | 1:30:A:ILE:HA    | 1:147:A:VAL:HG11 | 9        | 0.4           |
| (1,976)  | 1:13:A:ILE:HG22  | 1:17:A:ARG:HB2   | 8        | 0.4           |
| (1,955)  | 1:11:A:THR:HG21  | 1:9:A:THR:HA     | 8        | 0.4           |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 18       | 0.4           |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 19       | 0.4           |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB2  | 18       | 0.4           |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG22  | 5        | 0.4           |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG22  | 19       | 0.4           |
| (1,737)  | 1:132:A:GLN:H    | 1:132:A:GLN:HG2  | 7        | 0.4           |
| (1,659)  | 1:115:A:LYS:H    | 1:115:A:LYS:HG2  | 20       | 0.4           |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG12 | 6        | 0.4           |
| (1,610)  | 1:149:A:ALA:H    | 1:152:A:LEU:HD23 | 17       | 0.4           |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 9        | 0.4           |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 16       | 0.4           |
| (1,479)  | 1:87:A:GLU:H     | 1:68:A:LYS:HB3   | 17       | 0.4           |
| (1,479)  | 1:87:A:GLU:H     | 1:68:A:LYS:HB3   | 19       | 0.4           |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 8        | 0.4           |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 16       | 0.4           |
| (1,239)  | 1:42:A:GLU:H     | 1:55:A:LYS:HG2   | 8        | 0.4           |
| (1,216)  | 1:38:A:ILE:H     | 1:38:A:ILE:HG13  | 7        | 0.4           |
| (1,216)  | 1:38:A:ILE:H     | 1:38:A:ILE:HG13  | 19       | 0.4           |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 5        | 0.4           |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 17       | 0.4           |
| (1,96)   | 1:146:A:ALA:H    | 1:145:A:LYS:HB2  | 5        | 0.4           |
| (1,1696) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HB   | 3        | 0.39          |
| (1,1654) | 1:133:A:ILE:HG22 | 1:5:A:TYR:HB2    | 8        | 0.39          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 19       | 0.39          |
| (1,1588) | 1:105:A:VAL:HG13 | 1:105:A:VAL:H    | 4        | 0.39          |
| (1,1588) | 1:105:A:VAL:HG12 | 1:105:A:VAL:H    | 6        | 0.39          |
| (1,1543) | 1:156:A:ALA:HB1  | 1:154:A:ASN:HA   | 12       | 0.39          |
| (1,1530) | 1:45:A:GLU:HA    | 1:43:A:ILE:HG23  | 1        | 0.39          |
| (1,1530) | 1:45:A:GLU:HA    | 1:43:A:ILE:HG22  | 4        | 0.39          |
| (1,1510) | 1:84:A:THR:HG22  | 1:69:A:HIS:HA    | 12       | 0.39          |
| (1,1510) | 1:84:A:THR:HG22  | 1:69:A:HIS:HA    | 14       | 0.39          |
| (1,1510) | 1:84:A:THR:HG23  | 1:69:A:HIS:HA    | 18       | 0.39          |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD11  | 4        | 0.39          |
| (1,1301) | 1:44:A:ILE:HD11  | 1:53:A:ILE:HA    | 9        | 0.39          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG21  | 7        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1238) | 1:43:A:ILE:HD11  | 1:48:A:GLY:HA2   | 16       | 0.39          |
| (1,1233) | 1:133:A:ILE:HG13 | 1:128:A:ILE:HB   | 12       | 0.39          |
| (1,1204) | 1:38:A:ILE:HD13  | 1:58:A:PHE:HZ    | 12       | 0.39          |
| (1,1203) | 1:38:A:ILE:HD11  | 1:38:A:ILE:HA    | 4        | 0.39          |
| (1,1171) | 1:33:A:VAL:HG22  | 1:29:A:LEU:HB2   | 11       | 0.39          |
| (1,1134) | 1:30:A:ILE:HG21  | 1:37:A:ALA:HB3   | 9        | 0.39          |
| (1,1134) | 1:30:A:ILE:HG21  | 1:37:A:ALA:HB1   | 15       | 0.39          |
| (1,929)  | 1:9:A:THR:HG23   | 1:22:A:PHE:HD2   | 17       | 0.39          |
| (1,886)  | 1:2:A:VAL:HG23   | 1:119:A:LYS:HD2  | 13       | 0.39          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 7        | 0.39          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 18       | 0.39          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 11       | 0.39          |
| (1,777)  | 1:142:A:GLY:H    | 1:141:A:SER:HB3  | 14       | 0.39          |
| (1,505)  | 1:96:A:GLU:H     | 1:85:A:LEU:HD13  | 14       | 0.39          |
| (1,479)  | 1:87:A:GLU:H     | 1:68:A:LYS:HB3   | 3        | 0.39          |
| (1,375)  | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 15       | 0.39          |
| (1,216)  | 1:38:A:ILE:H     | 1:38:A:ILE:HG13  | 12       | 0.39          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 14       | 0.39          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 19       | 0.39          |
| (1,58)   | 1:9:A:THR:H      | 1:8:A:GLU:HG3    | 9        | 0.39          |
| (3,179)  | 1:148:A:GLU:HA   | 1:152:A:LEU:HD21 | 18       | 0.38          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2   | 5        | 0.38          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE2   | 8        | 0.38          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE1   | 10       | 0.38          |
| (1,1697) | 1:151:A:LEU:HD11 | 1:150:A:TYR:HD2  | 5        | 0.38          |
| (1,1697) | 1:151:A:LEU:HD11 | 1:150:A:TYR:HD1  | 7        | 0.38          |
| (1,1694) | 1:151:A:LEU:HD13 | 1:147:A:VAL:HA   | 4        | 0.38          |
| (1,1694) | 1:151:A:LEU:HD13 | 1:147:A:VAL:HA   | 14       | 0.38          |
| (1,1678) | 1:134:A:LYS:HA   | 1:134:A:LYS:HD3  | 19       | 0.38          |
| (1,1675) | 1:147:A:VAL:HG23 | 1:22:A:PHE:HB2   | 10       | 0.38          |
| (1,1588) | 1:105:A:VAL:HG11 | 1:105:A:VAL:H    | 15       | 0.38          |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG22 | 11       | 0.38          |
| (1,1530) | 1:45:A:GLU:HA    | 1:43:A:ILE:HG23  | 6        | 0.38          |
| (1,1514) | 1:18:A:LEU:HD23  | 1:13:A:ILE:HA    | 19       | 0.38          |
| (1,1510) | 1:84:A:THR:HG21  | 1:69:A:HIS:HA    | 3        | 0.38          |
| (1,1510) | 1:84:A:THR:HG21  | 1:69:A:HIS:HA    | 16       | 0.38          |
| (1,1336) | 1:128:A:ILE:HD11 | 1:120:A:TYR:HB2  | 7        | 0.38          |
| (1,1203) | 1:38:A:ILE:HD11  | 1:38:A:ILE:HA    | 1        | 0.38          |
| (1,1183) | 1:34:A:ALA:HB1   | 1:147:A:VAL:HG12 | 5        | 0.38          |
| (1,1183) | 1:34:A:ALA:HB2   | 1:147:A:VAL:HG11 | 10       | 0.38          |
| (1,1166) | 1:33:A:VAL:HG11  | 1:29:A:LEU:H     | 18       | 0.38          |
| (1,1154) | 1:96:A:GLU:HA    | 1:123:A:LYS:HD3  | 6        | 0.38          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1152) | 1:151:A:LEU:HA  | 1:150:A:TYR:HB2  | 19       | 0.38          |
| (1,1074) | 1:24:A:LEU:HA   | 1:43:A:ILE:HD12  | 6        | 0.38          |
| (1,1021) | 1:128:A:ILE:HA  | 1:127:A:GLU:HB2  | 20       | 0.38          |
| (1,994)  | 1:82:A:ALA:HB2  | 1:71:A:ILE:HA    | 14       | 0.38          |
| (1,976)  | 1:13:A:ILE:HG21 | 1:17:A:ARG:HB2   | 6        | 0.38          |
| (1,976)  | 1:13:A:ILE:HG23 | 1:17:A:ARG:HB2   | 17       | 0.38          |
| (1,890)  | 1:2:A:VAL:HG12  | 1:4:A:THR:HB     | 3        | 0.38          |
| (1,890)  | 1:2:A:VAL:HG11  | 1:4:A:THR:HB     | 20       | 0.38          |
| (1,882)  | 1:2:A:VAL:HG22  | 1:119:A:LYS:HE2  | 7        | 0.38          |
| (1,849)  | 1:17:A:ARG:HH11 | 1:155:A:PRO:HG3  | 7        | 0.38          |
| (1,826)  | 1:153:A:ALA:H   | 1:151:A:LEU:HB3  | 14       | 0.38          |
| (1,826)  | 1:153:A:ALA:H   | 1:151:A:LEU:HB3  | 17       | 0.38          |
| (1,812)  | 1:148:A:GLU:H   | 1:152:A:LEU:HD23 | 1        | 0.38          |
| (1,783)  | 1:151:A:LEU:H   | 1:150:A:TYR:HB2  | 13       | 0.38          |
| (1,586)  | 1:106:A:ALA:H   | 1:15:A:PRO:HG2   | 11       | 0.38          |
| (1,586)  | 1:106:A:ALA:H   | 1:15:A:PRO:HG2   | 14       | 0.38          |
| (1,505)  | 1:96:A:GLU:H    | 1:85:A:LEU:HD12  | 15       | 0.38          |
| (1,479)  | 1:87:A:GLU:H    | 1:68:A:LYS:HB3   | 6        | 0.38          |
| (1,476)  | 1:86:A:ILE:H    | 1:86:A:ILE:HG21  | 12       | 0.38          |
| (1,458)  | 1:82:A:ALA:H    | 1:73:A:GLU:HG3   | 17       | 0.38          |
| (1,191)  | 1:34:A:ALA:H    | 1:31:A:PRO:HD3   | 1        | 0.38          |
| (1,96)   | 1:146:A:ALA:H   | 1:145:A:LYS:HB2  | 3        | 0.38          |
| (1,96)   | 1:146:A:ALA:H   | 1:145:A:LYS:HB2  | 10       | 0.38          |
| (1,96)   | 1:146:A:ALA:H   | 1:145:A:LYS:HB2  | 18       | 0.38          |
| (1,95)   | 1:13:A:ILE:H    | 1:12:A:VAL:HG13  | 17       | 0.38          |
| (3,174)  | 1:55:A:LYS:HA   | 1:42:A:GLU:HB2   | 1        | 0.37          |
| (3,135)  | 1:115:A:LYS:HD3 | 1:8:A:GLU:HA     | 4        | 0.37          |
| (3,127)  | 1:5:A:TYR:HB2   | 1:6:A:GLU:HG2    | 9        | 0.37          |
| (3,127)  | 1:5:A:TYR:HB2   | 1:6:A:GLU:HG2    | 11       | 0.37          |
| (3,83)   | 1:55:A:LYS:HE2  | 1:55:A:LYS:HD2   | 1        | 0.37          |
| (3,83)   | 1:20:A:LYS:HD2  | 1:20:A:LYS:HE2   | 2        | 0.37          |
| (3,83)   | 1:55:A:LYS:HE2  | 1:55:A:LYS:HD2   | 4        | 0.37          |
| (3,83)   | 1:55:A:LYS:HE2  | 1:55:A:LYS:HD2   | 5        | 0.37          |
| (3,83)   | 1:55:A:LYS:HE2  | 1:55:A:LYS:HD2   | 6        | 0.37          |
| (3,83)   | 1:55:A:LYS:HE2  | 1:55:A:LYS:HD2   | 7        | 0.37          |
| (3,83)   | 1:20:A:LYS:HD2  | 1:20:A:LYS:HE2   | 8        | 0.37          |
| (3,83)   | 1:20:A:LYS:HD2  | 1:20:A:LYS:HE2   | 9        | 0.37          |
| (3,83)   | 1:55:A:LYS:HE2  | 1:55:A:LYS:HD2   | 10       | 0.37          |
| (3,83)   | 1:20:A:LYS:HD2  | 1:20:A:LYS:HE2   | 11       | 0.37          |
| (3,83)   | 1:55:A:LYS:HE2  | 1:55:A:LYS:HD2   | 12       | 0.37          |
| (3,83)   | 1:55:A:LYS:HE2  | 1:55:A:LYS:HD2   | 14       | 0.37          |
| (3,83)   | 1:20:A:LYS:HD2  | 1:20:A:LYS:HE2   | 17       | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,83)   | 1:20:A:LYS:HD2   | 1:20:A:LYS:HE2   | 20       | 0.37          |
| (1,1623) | 1:117:A:THR:HB   | 1:101:A:GLU:HB3  | 18       | 0.37          |
| (1,1607) | 1:111:A:GLY:HA3  | 1:14:A:THR:HG21  | 13       | 0.37          |
| (1,1607) | 1:111:A:GLY:HA3  | 1:14:A:THR:HG21  | 20       | 0.37          |
| (1,1588) | 1:105:A:VAL:HG12 | 1:105:A:VAL:H    | 2        | 0.37          |
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG22 | 20       | 0.37          |
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG23  | 2        | 0.37          |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD13  | 15       | 0.37          |
| (1,1510) | 1:84:A:THR:HG23  | 1:69:A:HIS:HA    | 5        | 0.37          |
| (1,1510) | 1:84:A:THR:HG23  | 1:69:A:HIS:HA    | 10       | 0.37          |
| (1,1510) | 1:84:A:THR:HG22  | 1:69:A:HIS:HA    | 13       | 0.37          |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD13  | 17       | 0.37          |
| (1,1271) | 1:48:A:GLY:HA2   | 1:71:A:ILE:HG12  | 4        | 0.37          |
| (1,1238) | 1:43:A:ILE:HD13  | 1:48:A:GLY:HA2   | 5        | 0.37          |
| (1,1204) | 1:38:A:ILE:HD13  | 1:58:A:PHE:HZ    | 1        | 0.37          |
| (1,1203) | 1:38:A:ILE:HD12  | 1:38:A:ILE:HA    | 9        | 0.37          |
| (1,1203) | 1:38:A:ILE:HD11  | 1:38:A:ILE:HA    | 20       | 0.37          |
| (1,1183) | 1:34:A:ALA:HB3   | 1:147:A:VAL:HG12 | 15       | 0.37          |
| (1,1166) | 1:33:A:VAL:HG12  | 1:29:A:LEU:H     | 15       | 0.37          |
| (1,1134) | 1:30:A:ILE:HG21  | 1:37:A:ALA:HB2   | 5        | 0.37          |
| (1,1134) | 1:30:A:ILE:HG22  | 1:37:A:ALA:HB2   | 18       | 0.37          |
| (1,995)  | 1:82:A:ALA:HB2   | 1:81:A:TYR:HB2   | 5        | 0.37          |
| (1,995)  | 1:82:A:ALA:HB3   | 1:81:A:TYR:HB2   | 11       | 0.37          |
| (1,939)  | 1:80:A:THR:HG21  | 1:74:A:ILE:HA    | 6        | 0.37          |
| (1,929)  | 1:9:A:THR:HG23   | 1:22:A:PHE:HD2   | 5        | 0.37          |
| (1,882)  | 1:2:A:VAL:HG21   | 1:119:A:LYS:HE2  | 20       | 0.37          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 9        | 0.37          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 12       | 0.37          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 4        | 0.37          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 7        | 0.37          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 1        | 0.37          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 16       | 0.37          |
| (1,777)  | 1:142:A:GLY:H    | 1:141:A:SER:HB3  | 16       | 0.37          |
| (1,752)  | 1:133:A:ILE:H    | 1:98:A:ILE:HG22  | 14       | 0.37          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD12  | 1        | 0.37          |
| (1,625)  | 1:111:A:GLY:H    | 1:109:A:ASP:HA   | 20       | 0.37          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 10       | 0.37          |
| (3,167)  | 1:146:A:ALA:HB2  | 1:35:A:PRO:HD2   | 15       | 0.36          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 17       | 0.36          |
| (3,58)   | 1:121:A:HIS:H    | 1:91:A:ILE:HD12  | 3        | 0.36          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE1   | 18       | 0.36          |
| (1,1701) | 1:153:A:ALA:HB3  | 1:154:A:ASN:HD22 | 17       | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1653) | 1:133:A:ILE:HG13 | 1:3:A:PHE:HD1    | 3        | 0.36          |
| (1,1618) | 1:114:A:LEU:HD22 | 1:9:A:THR:HB     | 15       | 0.36          |
| (1,1512) | 1:84:A:THR:HG21  | 1:71:A:ILE:HA    | 20       | 0.36          |
| (1,1510) | 1:84:A:THR:HG23  | 1:69:A:HIS:HA    | 20       | 0.36          |
| (1,1429) | 1:104:A:LEU:HD12 | 1:106:A:ALA:H    | 2        | 0.36          |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD13  | 6        | 0.36          |
| (1,1271) | 1:48:A:GLY:HA2   | 1:71:A:ILE:HG12  | 11       | 0.36          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG21  | 17       | 0.36          |
| (1,1203) | 1:38:A:ILE:HD13  | 1:38:A:ILE:HA    | 15       | 0.36          |
| (1,1183) | 1:34:A:ALA:HB3   | 1:147:A:VAL:HG12 | 7        | 0.36          |
| (1,1183) | 1:34:A:ALA:HB1   | 1:147:A:VAL:HG11 | 13       | 0.36          |
| (1,1171) | 1:33:A:VAL:HG23  | 1:29:A:LEU:HB2   | 20       | 0.36          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 2        | 0.36          |
| (1,1141) | 1:102:A:ILE:HG23 | 1:116:A:SER:HB3  | 14       | 0.36          |
| (1,995)  | 1:82:A:ALA:HB3   | 1:81:A:TYR:HB2   | 13       | 0.36          |
| (1,994)  | 1:82:A:ALA:HB3   | 1:71:A:ILE:HA    | 10       | 0.36          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 10       | 0.36          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 14       | 0.36          |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3  | 6        | 0.36          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 9        | 0.36          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 19       | 0.36          |
| (1,479)  | 1:87:A:GLU:H     | 1:68:A:LYS:HB3   | 12       | 0.36          |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB2   | 10       | 0.36          |
| (1,96)   | 1:146:A:ALA:H    | 1:145:A:LYS:HB2  | 8        | 0.36          |
| (1,58)   | 1:9:A:THR:H      | 1:8:A:GLU:HG3    | 3        | 0.36          |
| (3,153)  | 1:113:A:ILE:HD13 | 1:108:A:PRO:HG2  | 12       | 0.35          |
| (3,151)  | 1:104:A:LEU:HD21 | 1:18:A:LEU:HB3   | 1        | 0.35          |
| (3,135)  | 1:115:A:LYS:HD3  | 1:8:A:GLU:HA     | 10       | 0.35          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 12       | 0.35          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE2   | 2        | 0.35          |
| (1,1694) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HA   | 20       | 0.35          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG22 | 7        | 0.35          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG21 | 10       | 0.35          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG23 | 15       | 0.35          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG23 | 18       | 0.35          |
| (1,1660) | 1:143:A:ILE:HA   | 1:144:A:PHE:HD2  | 8        | 0.35          |
| (1,1589) | 1:105:A:VAL:HG13 | 1:107:A:SER:H    | 9        | 0.35          |
| (1,1579) | 1:104:A:LEU:HA   | 1:104:A:LEU:HG   | 5        | 0.35          |
| (1,1579) | 1:104:A:LEU:HA   | 1:104:A:LEU:HG   | 9        | 0.35          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 19       | 0.35          |
| (1,1530) | 1:45:A:GLU:HA    | 1:43:A:ILE:HG23  | 20       | 0.35          |
| (1,1514) | 1:18:A:LEU:HD22  | 1:13:A:ILE:HA    | 1        | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1514) | 1:18:A:LEU:HD21  | 1:13:A:ILE:HA    | 5        | 0.35          |
| (1,1512) | 1:84:A:THR:HG23  | 1:71:A:ILE:HA    | 14       | 0.35          |
| (1,1510) | 1:84:A:THR:HG23  | 1:69:A:HIS:HA    | 9        | 0.35          |
| (1,1450) | 1:71:A:ILE:HG22  | 1:70:A:ARG:HE    | 14       | 0.35          |
| (1,1289) | 1:52:A:THR:HB    | 1:71:A:ILE:HG21  | 18       | 0.35          |
| (1,1238) | 1:43:A:ILE:HD13  | 1:48:A:GLY:HA2   | 2        | 0.35          |
| (1,1238) | 1:43:A:ILE:HD11  | 1:48:A:GLY:HA2   | 14       | 0.35          |
| (1,1203) | 1:38:A:ILE:HD12  | 1:38:A:ILE:HA    | 8        | 0.35          |
| (1,1203) | 1:38:A:ILE:HD13  | 1:38:A:ILE:HA    | 17       | 0.35          |
| (1,1183) | 1:34:A:ALA:HB2   | 1:147:A:VAL:HG11 | 19       | 0.35          |
| (1,1030) | 1:55:A:LYS:HE3   | 1:44:A:ILE:HD12  | 10       | 0.35          |
| (1,929)  | 1:9:A:THR:HG22   | 1:22:A:PHE:HD1   | 11       | 0.35          |
| (1,882)  | 1:2:A:VAL:HG22   | 1:119:A:LYS:HE2  | 16       | 0.35          |
| (1,870)  | 1:145:A:LYS:H    | 1:144:A:PHE:HB2  | 14       | 0.35          |
| (1,849)  | 1:17:A:ARG:HH11  | 1:155:A:PRO:HG3  | 5        | 0.35          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 16       | 0.35          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD12  | 11       | 0.35          |
| (1,625)  | 1:111:A:GLY:H    | 1:109:A:ASP:HA   | 7        | 0.35          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD21  | 11       | 0.35          |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 17       | 0.35          |
| (1,481)  | 1:87:A:GLU:H     | 1:85:A:LEU:HB2   | 14       | 0.35          |
| (1,233)  | 1:70:A:ARG:HH22  | 1:70:A:ARG:HB2   | 2        | 0.35          |
| (1,233)  | 1:70:A:ARG:HH22  | 1:70:A:ARG:HB2   | 17       | 0.35          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 4        | 0.35          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 15       | 0.35          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB3   | 10       | 0.35          |
| (3,167)  | 1:146:A:ALA:HB3  | 1:35:A:PRO:HD2   | 4        | 0.34          |
| (3,158)  | 1:118:A:SER:HB2  | 1:6:A:GLU:HG2    | 18       | 0.34          |
| (1,1696) | 1:151:A:LEU:HD13 | 1:147:A:VAL:HB   | 6        | 0.34          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG21 | 1        | 0.34          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG22 | 5        | 0.34          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG21 | 17       | 0.34          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 13       | 0.34          |
| (1,1592) | 1:106:A:ALA:HA   | 1:15:A:PRO:HG2   | 19       | 0.34          |
| (1,1589) | 1:105:A:VAL:HG12 | 1:107:A:SER:H    | 6        | 0.34          |
| (1,1589) | 1:105:A:VAL:HG11 | 1:107:A:SER:H    | 10       | 0.34          |
| (1,1579) | 1:104:A:LEU:HA   | 1:104:A:LEU:HG   | 8        | 0.34          |
| (1,1579) | 1:104:A:LEU:HA   | 1:104:A:LEU:HG   | 13       | 0.34          |
| (1,1516) | 1:133:A:ILE:HG22 | 1:5:A:TYR:HE2    | 10       | 0.34          |
| (1,1514) | 1:18:A:LEU:HD22  | 1:13:A:ILE:HA    | 14       | 0.34          |
| (1,1461) | 1:74:A:ILE:HG23  | 1:76:A:ASN:H     | 12       | 0.34          |
| (1,1450) | 1:71:A:ILE:HG21  | 1:70:A:ARG:HE    | 8        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1450) | 1:71:A:ILE:HG22  | 1:70:A:ARG:HE    | 10       | 0.34          |
| (1,1426) | 1:116:A:SER:HA   | 1:115:A:LYS:HB2  | 20       | 0.34          |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD13  | 14       | 0.34          |
| (1,1383) | 1:130:A:GLU:HG2  | 1:133:A:ILE:HG12 | 8        | 0.34          |
| (1,1271) | 1:48:A:GLY:HA2   | 1:71:A:ILE:HG12  | 3        | 0.34          |
| (1,1183) | 1:34:A:ALA:HB1   | 1:147:A:VAL:HG13 | 9        | 0.34          |
| (1,1166) | 1:33:A:VAL:HG12  | 1:29:A:LEU:H     | 19       | 0.34          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 4        | 0.34          |
| (1,1134) | 1:30:A:ILE:HG23  | 1:37:A:ALA:HB3   | 3        | 0.34          |
| (1,1134) | 1:30:A:ILE:HG22  | 1:37:A:ALA:HB1   | 4        | 0.34          |
| (1,1134) | 1:30:A:ILE:HG21  | 1:37:A:ALA:HB3   | 6        | 0.34          |
| (1,1134) | 1:30:A:ILE:HG22  | 1:37:A:ALA:HB2   | 19       | 0.34          |
| (1,994)  | 1:82:A:ALA:HB1   | 1:71:A:ILE:HA    | 1        | 0.34          |
| (1,994)  | 1:82:A:ALA:HB2   | 1:71:A:ILE:HA    | 4        | 0.34          |
| (1,890)  | 1:2:A:VAL:HG13   | 1:4:A:THR:HB     | 16       | 0.34          |
| (1,885)  | 1:2:A:VAL:HG21   | 1:4:A:THR:HG23   | 2        | 0.34          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 17       | 0.34          |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG12 | 20       | 0.34          |
| (1,586)  | 1:106:A:ALA:H    | 1:15:A:PRO:HG2   | 4        | 0.34          |
| (1,519)  | 1:97:A:LYS:H     | 1:91:A:ILE:HD12  | 10       | 0.34          |
| (1,479)  | 1:87:A:GLU:H     | 1:68:A:LYS:HB3   | 4        | 0.34          |
| (1,479)  | 1:87:A:GLU:H     | 1:68:A:LYS:HB3   | 18       | 0.34          |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 6        | 0.34          |
| (1,265)  | 1:46:A:GLY:H     | 1:43:A:ILE:HG23  | 1        | 0.34          |
| (1,233)  | 1:70:A:ARG:HH22  | 1:70:A:ARG:HB2   | 1        | 0.34          |
| (1,233)  | 1:70:A:ARG:HH22  | 1:70:A:ARG:HB2   | 10       | 0.34          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 2        | 0.34          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 9        | 0.34          |
| (3,179)  | 1:148:A:GLU:HA   | 1:152:A:LEU:HD23 | 15       | 0.33          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 15       | 0.33          |
| (1,1696) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HB   | 16       | 0.33          |
| (1,1694) | 1:151:A:LEU:HD13 | 1:147:A:VAL:HA   | 5        | 0.33          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG22 | 3        | 0.33          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG21 | 6        | 0.33          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG22 | 9        | 0.33          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG23 | 14       | 0.33          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG22 | 16       | 0.33          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG23 | 19       | 0.33          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG22 | 20       | 0.33          |
| (1,1661) | 1:143:A:ILE:HA   | 1:37:A:ALA:HB3   | 13       | 0.33          |
| (1,1625) | 1:118:A:SER:HB2  | 1:99:A:ALA:HB2   | 8        | 0.33          |
| (1,1589) | 1:105:A:VAL:HG11 | 1:107:A:SER:H    | 7        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1579) | 1:104:A:LEU:HA   | 1:104:A:LEU:HG   | 11       | 0.33          |
| (1,1579) | 1:104:A:LEU:HA   | 1:104:A:LEU:HG   | 18       | 0.33          |
| (1,1574) | 1:128:A:ILE:HD12 | 1:91:A:ILE:HD12  | 6        | 0.33          |
| (1,1574) | 1:128:A:ILE:HD13 | 1:91:A:ILE:HD13  | 15       | 0.33          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 2        | 0.33          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 3        | 0.33          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 17       | 0.33          |
| (1,1335) | 1:128:A:ILE:HD13 | 1:128:A:ILE:HA   | 9        | 0.33          |
| (1,1304) | 1:56:A:ILE:HD11  | 1:27:A:ASP:HA    | 8        | 0.33          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG22  | 8        | 0.33          |
| (1,1203) | 1:38:A:ILE:HD13  | 1:38:A:ILE:HA    | 11       | 0.33          |
| (1,1183) | 1:34:A:ALA:HB2   | 1:147:A:VAL:HG12 | 18       | 0.33          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 13       | 0.33          |
| (1,1141) | 1:102:A:ILE:HG21 | 1:116:A:SER:HB3  | 19       | 0.33          |
| (1,1120) | 1:74:A:ILE:HD13  | 1:71:A:ILE:HA    | 20       | 0.33          |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD12  | 3        | 0.33          |
| (1,1023) | 1:17:A:ARG:HA    | 1:20:A:LYS:HE3   | 12       | 0.33          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 11       | 0.33          |
| (1,995)  | 1:82:A:ALA:HB3   | 1:81:A:TYR:HB2   | 4        | 0.33          |
| (1,995)  | 1:82:A:ALA:HB2   | 1:81:A:TYR:HB2   | 8        | 0.33          |
| (1,995)  | 1:82:A:ALA:HB3   | 1:81:A:TYR:HB2   | 18       | 0.33          |
| (1,976)  | 1:13:A:ILE:HG22  | 1:17:A:ARG:HB2   | 14       | 0.33          |
| (1,976)  | 1:13:A:ILE:HG21  | 1:17:A:ARG:HB2   | 20       | 0.33          |
| (1,904)  | 1:4:A:THR:HG21   | 1:6:A:GLU:HG3    | 17       | 0.33          |
| (1,890)  | 1:2:A:VAL:HG11   | 1:4:A:THR:HB     | 5        | 0.33          |
| (1,828)  | 1:153:A:ALA:H    | 1:149:A:ALA:HB2  | 16       | 0.33          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 4        | 0.33          |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 17       | 0.33          |
| (1,625)  | 1:111:A:GLY:H    | 1:109:A:ASP:HA   | 5        | 0.33          |
| (1,479)  | 1:87:A:GLU:H     | 1:68:A:LYS:HB3   | 7        | 0.33          |
| (1,477)  | 1:87:A:GLU:H     | 1:67:A:VAL:HG23  | 8        | 0.33          |
| (1,233)  | 1:70:A:ARG:HH22  | 1:70:A:ARG:HB2   | 18       | 0.33          |
| (1,181)  | 1:33:A:VAL:H     | 1:147:A:VAL:HG11 | 8        | 0.33          |
| (3,179)  | 1:148:A:GLU:HA   | 1:18:A:LEU:HD22  | 13       | 0.32          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2   | 12       | 0.32          |
| (3,151)  | 1:104:A:LEU:HD21 | 1:114:A:LEU:HG   | 7        | 0.32          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 2        | 0.32          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE1   | 5        | 0.32          |
| (3,9)    | 1:14:A:THR:H     | 1:111:A:GLY:HA2  | 8        | 0.32          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 15       | 0.32          |
| (1,1701) | 1:153:A:ALA:HB2  | 1:154:A:ASN:HD22 | 7        | 0.32          |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG22 | 11       | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1663) | 1:13:A:ILE:HD13  | 1:148:A:GLU:HA   | 11       | 0.32          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 3        | 0.32          |
| (1,1624) | 1:118:A:SER:HB2  | 1:119:A:LYS:HB2  | 17       | 0.32          |
| (1,1589) | 1:105:A:VAL:HG11 | 1:107:A:SER:H    | 5        | 0.32          |
| (1,1589) | 1:105:A:VAL:HG11 | 1:107:A:SER:H    | 11       | 0.32          |
| (1,1589) | 1:105:A:VAL:HG12 | 1:107:A:SER:H    | 20       | 0.32          |
| (1,1579) | 1:104:A:LEU:HA   | 1:104:A:LEU:HG   | 1        | 0.32          |
| (1,1579) | 1:104:A:LEU:HA   | 1:104:A:LEU:HG   | 19       | 0.32          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 12       | 0.32          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 14       | 0.32          |
| (1,1514) | 1:18:A:LEU:HD23  | 1:13:A:ILE:HA    | 4        | 0.32          |
| (1,1450) | 1:71:A:ILE:HG23  | 1:70:A:ARG:HE    | 11       | 0.32          |
| (1,1446) | 1:56:A:ILE:HD11  | 1:40:A:SER:HA    | 6        | 0.32          |
| (1,1351) | 1:56:A:ILE:HG22  | 1:38:A:ILE:HG21  | 10       | 0.32          |
| (1,1259) | 1:8:A:GLU:HG3    | 1:114:A:LEU:H    | 3        | 0.32          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG23  | 14       | 0.32          |
| (1,1183) | 1:34:A:ALA:HB1   | 1:147:A:VAL:HG13 | 6        | 0.32          |
| (1,1183) | 1:34:A:ALA:HB3   | 1:147:A:VAL:HG11 | 14       | 0.32          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 8        | 0.32          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 9        | 0.32          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 16       | 0.32          |
| (1,1141) | 1:102:A:ILE:HG23 | 1:116:A:SER:HB3  | 13       | 0.32          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD12 | 2        | 0.32          |
| (1,1023) | 1:17:A:ARG:HA    | 1:20:A:LYS:HE3   | 3        | 0.32          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 8        | 0.32          |
| (1,929)  | 1:9:A:THR:HG21   | 1:22:A:PHE:HD1   | 3        | 0.32          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 9        | 0.32          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 18       | 0.32          |
| (1,711)  | 1:123:A:LYS:H    | 1:95:A:LEU:HD13  | 17       | 0.32          |
| (1,659)  | 1:115:A:LYS:H    | 1:115:A:LYS:HG2  | 19       | 0.32          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 10       | 0.32          |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 3        | 0.32          |
| (1,96)   | 1:146:A:ALA:H    | 1:145:A:LYS:HB2  | 4        | 0.32          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB2   | 3        | 0.32          |
| (3,172)  | 1:101:A:GLU:HA   | 1:81:A:TYR:H     | 7        | 0.31          |
| (3,167)  | 1:146:A:ALA:HB2  | 1:35:A:PRO:HD3   | 3        | 0.31          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE2   | 14       | 0.31          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 12       | 0.31          |
| (1,1771) | 1:150:A:TYR:HA   | 1:154:A:ASN:HD22 | 5        | 0.31          |
| (1,1762) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD23 | 3        | 0.31          |
| (1,1696) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HB   | 5        | 0.31          |
| (1,1694) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HA   | 3        | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG23 | 13       | 0.31          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 17       | 0.31          |
| (1,1626) | 1:118:A:SER:HB2  | 1:117:A:THR:HG23 | 6        | 0.31          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 8        | 0.31          |
| (1,1610) | 1:112:A:SER:HA   | 1:15:A:PRO:HG2   | 14       | 0.31          |
| (1,1607) | 1:111:A:GLY:HA3  | 1:14:A:THR:HG22  | 9        | 0.31          |
| (1,1589) | 1:105:A:VAL:HG11 | 1:107:A:SER:H    | 1        | 0.31          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 3        | 0.31          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 16       | 0.31          |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG22  | 2        | 0.31          |
| (1,1238) | 1:43:A:ILE:HD12  | 1:48:A:GLY:HA2   | 9        | 0.31          |
| (1,1141) | 1:102:A:ILE:HG22 | 1:116:A:SER:HB3  | 7        | 0.31          |
| (1,1134) | 1:30:A:ILE:HG21  | 1:37:A:ALA:HB3   | 2        | 0.31          |
| (1,1134) | 1:30:A:ILE:HG21  | 1:37:A:ALA:HB3   | 14       | 0.31          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD13 | 16       | 0.31          |
| (1,1043) | 1:18:A:LEU:HD23  | 1:22:A:PHE:HD2   | 8        | 0.31          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 10       | 0.31          |
| (1,976)  | 1:13:A:ILE:HG23  | 1:17:A:ARG:HB2   | 3        | 0.31          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 15       | 0.31          |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 5        | 0.31          |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3  | 4        | 0.31          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 14       | 0.31          |
| (1,642)  | 1:113:A:ILE:H    | 1:105:A:VAL:HG11 | 7        | 0.31          |
| (1,625)  | 1:111:A:GLY:H    | 1:109:A:ASP:HA   | 1        | 0.31          |
| (1,625)  | 1:111:A:GLY:H    | 1:109:A:ASP:HA   | 4        | 0.31          |
| (1,625)  | 1:111:A:GLY:H    | 1:109:A:ASP:HA   | 9        | 0.31          |
| (1,535)  | 1:100:A:TYR:H    | 1:83:A:CYS:HB3   | 18       | 0.31          |
| (1,477)  | 1:87:A:GLU:H     | 1:67:A:VAL:HG22  | 9        | 0.31          |
| (1,477)  | 1:87:A:GLU:H     | 1:67:A:VAL:HG22  | 15       | 0.31          |
| (1,476)  | 1:86:A:ILE:H     | 1:86:A:ILE:HG21  | 5        | 0.31          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB2   | 5        | 0.31          |
| (1,40)   | 1:5:A:TYR:H      | 1:119:A:LYS:HG2  | 10       | 0.31          |
| (3,157)  | 1:114:A:LEU:HD22 | 1:22:A:PHE:HE2   | 6        | 0.3           |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE2   | 19       | 0.3           |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 1        | 0.3           |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 19       | 0.3           |
| (1,1696) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HB   | 14       | 0.3           |
| (1,1696) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HB   | 15       | 0.3           |
| (1,1678) | 1:134:A:LYS:HA   | 1:134:A:LYS:HD3  | 15       | 0.3           |
| (1,1671) | 1:147:A:VAL:HA   | 1:147:A:VAL:HG23 | 4        | 0.3           |
| (1,1589) | 1:105:A:VAL:HG12 | 1:107:A:SER:H    | 8        | 0.3           |
| (1,1589) | 1:105:A:VAL:HG11 | 1:107:A:SER:H    | 18       | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1576) | 1:103:A:LYS:HE3  | 1:105:A:VAL:HG22 | 13       | 0.3           |
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG21  | 4        | 0.3           |
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG21  | 8        | 0.3           |
| (1,1557) | 1:85:A:LEU:HD11  | 1:91:A:ILE:HG12  | 1        | 0.3           |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 7        | 0.3           |
| (1,1541) | 1:143:A:ILE:HA   | 1:30:A:ILE:HG12  | 20       | 0.3           |
| (1,1537) | 1:128:A:ILE:HD13 | 1:120:A:TYR:HB3  | 14       | 0.3           |
| (1,1514) | 1:18:A:LEU:HD21  | 1:13:A:ILE:HA    | 7        | 0.3           |
| (1,1461) | 1:74:A:ILE:HG21  | 1:76:A:ASN:H     | 20       | 0.3           |
| (1,1429) | 1:104:A:LEU:HD12 | 1:106:A:ALA:H    | 17       | 0.3           |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD12  | 7        | 0.3           |
| (1,1351) | 1:56:A:ILE:HG23  | 1:38:A:ILE:HG22  | 8        | 0.3           |
| (1,1289) | 1:52:A:THR:HB    | 1:71:A:ILE:HG22  | 20       | 0.3           |
| (1,1271) | 1:48:A:GLY:HA2   | 1:71:A:ILE:HG12  | 20       | 0.3           |
| (1,1242) | 1:53:A:ILE:HG12  | 1:44:A:ILE:HG23  | 9        | 0.3           |
| (1,1183) | 1:34:A:ALA:HB1   | 1:147:A:VAL:HG12 | 11       | 0.3           |
| (1,1168) | 1:33:A:VAL:HG11  | 1:150:A:TYR:HB3  | 15       | 0.3           |
| (1,1127) | 1:71:A:ILE:HG22  | 1:82:A:ALA:HA    | 5        | 0.3           |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD13 | 6        | 0.3           |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 12       | 0.3           |
| (1,995)  | 1:82:A:ALA:HB2   | 1:81:A:TYR:HB2   | 19       | 0.3           |
| (1,976)  | 1:13:A:ILE:HG23  | 1:17:A:ARG:HB2   | 4        | 0.3           |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 4        | 0.3           |
| (1,783)  | 1:151:A:LEU:H    | 1:150:A:TYR:HB2  | 6        | 0.3           |
| (1,614)  | 1:110:A:GLY:H    | 1:106:A:ALA:HB3  | 16       | 0.3           |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD22  | 10       | 0.3           |
| (1,493)  | 1:90:A:ALA:H     | 1:67:A:VAL:HG12  | 6        | 0.3           |
| (1,476)  | 1:86:A:ILE:H     | 1:86:A:ILE:HG23  | 6        | 0.3           |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 1        | 0.3           |
| (1,239)  | 1:42:A:GLU:H     | 1:55:A:LYS:HG2   | 7        | 0.3           |
| (1,191)  | 1:34:A:ALA:H     | 1:31:A:PRO:HD3   | 6        | 0.3           |
| (1,96)   | 1:146:A:ALA:H    | 1:145:A:LYS:HB2  | 13       | 0.3           |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB2   | 12       | 0.3           |
| (3,172)  | 1:101:A:GLU:HA   | 1:81:A:TYR:H     | 3        | 0.29          |
| (3,151)  | 1:104:A:LEU:HD22 | 1:18:A:LEU:HB3   | 11       | 0.29          |
| (3,151)  | 1:104:A:LEU:HD22 | 1:114:A:LEU:HG   | 20       | 0.29          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 5        | 0.29          |
| (1,1697) | 1:151:A:LEU:HD12 | 1:150:A:TYR:HD2  | 16       | 0.29          |
| (1,1694) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HA   | 19       | 0.29          |
| (1,1678) | 1:134:A:LYS:HA   | 1:134:A:LYS:HD3  | 8        | 0.29          |
| (1,1675) | 1:147:A:VAL:HG23 | 1:22:A:PHE:HB2   | 1        | 0.29          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 6        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1589) | 1:105:A:VAL:HG12 | 1:107:A:SER:H    | 13       | 0.29          |
| (1,1589) | 1:105:A:VAL:HG13 | 1:107:A:SER:H    | 16       | 0.29          |
| (1,1579) | 1:104:A:LEU:HA   | 1:104:A:LEU:HG   | 10       | 0.29          |
| (1,1556) | 1:104:A:LEU:HD11 | 1:79:A:PHE:HB3   | 19       | 0.29          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 15       | 0.29          |
| (1,1537) | 1:128:A:ILE:HD11 | 1:120:A:TYR:HB3  | 12       | 0.29          |
| (1,1510) | 1:84:A:THR:HG21  | 1:69:A:HIS:HA    | 6        | 0.29          |
| (1,1461) | 1:74:A:ILE:HG22  | 1:76:A:ASN:H     | 2        | 0.29          |
| (1,1461) | 1:74:A:ILE:HG23  | 1:76:A:ASN:H     | 4        | 0.29          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 14       | 0.29          |
| (1,1328) | 1:104:A:LEU:HD12 | 1:112:A:SER:HB3  | 2        | 0.29          |
| (1,1312) | 1:44:A:ILE:HG12  | 1:55:A:LYS:HE3   | 18       | 0.29          |
| (1,1300) | 1:71:A:ILE:HD12  | 1:70:A:ARG:HE    | 19       | 0.29          |
| (1,1183) | 1:34:A:ALA:HB3   | 1:147:A:VAL:HG11 | 1        | 0.29          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 8        | 0.29          |
| (1,1166) | 1:33:A:VAL:HG13  | 1:29:A:LEU:H     | 14       | 0.29          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 15       | 0.29          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 20       | 0.29          |
| (1,1134) | 1:30:A:ILE:HG23  | 1:37:A:ALA:HB1   | 1        | 0.29          |
| (1,1134) | 1:30:A:ILE:HG22  | 1:37:A:ALA:HB3   | 16       | 0.29          |
| (1,1127) | 1:71:A:ILE:HG21  | 1:82:A:ALA:HA    | 13       | 0.29          |
| (1,1087) | 1:26:A:ALA:HB1   | 1:23:A:VAL:HA    | 14       | 0.29          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 17       | 0.29          |
| (1,995)  | 1:82:A:ALA:HB3   | 1:81:A:TYR:HB2   | 12       | 0.29          |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG22  | 10       | 0.29          |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG22  | 15       | 0.29          |
| (1,905)  | 1:4:A:THR:HG21   | 1:119:A:LYS:HB2  | 4        | 0.29          |
| (1,870)  | 1:145:A:LYS:H    | 1:144:A:PHE:HB2  | 5        | 0.29          |
| (1,859)  | 1:78:A:ASN:HD21  | 1:77:A:ALA:HB2   | 12       | 0.29          |
| (1,839)  | 1:154:A:ASN:H    | 1:153:A:ALA:HB2  | 8        | 0.29          |
| (1,762)  | 1:139:A:GLU:H    | 1:135:A:ALA:HB2  | 19       | 0.29          |
| (1,625)  | 1:111:A:GLY:H    | 1:109:A:ASP:HA   | 13       | 0.29          |
| (1,625)  | 1:111:A:GLY:H    | 1:109:A:ASP:HA   | 14       | 0.29          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 15       | 0.29          |
| (1,233)  | 1:70:A:ARG:HH22  | 1:70:A:ARG:HB2   | 4        | 0.29          |
| (1,181)  | 1:33:A:VAL:H     | 1:147:A:VAL:HG11 | 2        | 0.29          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB1   | 8        | 0.29          |
| (1,71)   | 1:30:A:ILE:H     | 1:30:A:ILE:HG12  | 17       | 0.29          |
| (3,172)  | 1:101:A:GLU:HA   | 1:81:A:TYR:H     | 20       | 0.28          |
| (3,153)  | 1:113:A:ILE:HD12 | 1:108:A:PRO:HG2  | 17       | 0.28          |
| (3,151)  | 1:104:A:LEU:HD23 | 1:114:A:LEU:HG   | 5        | 0.28          |
| (3,151)  | 1:104:A:LEU:HD21 | 1:18:A:LEU:HB3   | 10       | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 7        | 0.28          |
| (3,58)   | 1:121:A:HIS:H    | 1:128:A:ILE:HG12 | 6        | 0.28          |
| (1,1660) | 1:143:A:ILE:HA   | 1:144:A:PHE:HD2  | 5        | 0.28          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 16       | 0.28          |
| (1,1589) | 1:105:A:VAL:HG13 | 1:107:A:SER:H    | 4        | 0.28          |
| (1,1589) | 1:105:A:VAL:HG13 | 1:107:A:SER:H    | 19       | 0.28          |
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG22  | 1        | 0.28          |
| (1,1574) | 1:128:A:ILE:HD13 | 1:91:A:ILE:HD12  | 2        | 0.28          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 1        | 0.28          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 4        | 0.28          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 9        | 0.28          |
| (1,1514) | 1:18:A:LEU:HD21  | 1:13:A:ILE:HA    | 17       | 0.28          |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD12  | 13       | 0.28          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 7        | 0.28          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 5        | 0.28          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 10       | 0.28          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 17       | 0.28          |
| (1,1141) | 1:102:A:ILE:HG21 | 1:116:A:SER:HB3  | 18       | 0.28          |
| (1,1134) | 1:30:A:ILE:HG21  | 1:37:A:ALA:HB2   | 17       | 0.28          |
| (1,995)  | 1:82:A:ALA:HB3   | 1:81:A:TYR:HB2   | 9        | 0.28          |
| (1,995)  | 1:82:A:ALA:HB2   | 1:81:A:TYR:HB2   | 17       | 0.28          |
| (1,994)  | 1:82:A:ALA:HB2   | 1:71:A:ILE:HA    | 12       | 0.28          |
| (1,983)  | 1:14:A:THR:HA    | 1:111:A:GLY:HA3  | 15       | 0.28          |
| (1,957)  | 1:11:A:THR:HG21  | 1:112:A:SER:HB2  | 3        | 0.28          |
| (1,939)  | 1:80:A:THR:HG21  | 1:74:A:ILE:HA    | 4        | 0.28          |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG21  | 13       | 0.28          |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG22  | 16       | 0.28          |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG23  | 18       | 0.28          |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG23  | 19       | 0.28          |
| (1,873)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:HA   | 11       | 0.28          |
| (1,859)  | 1:78:A:ASN:HD21  | 1:77:A:ALA:HB1   | 4        | 0.28          |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3  | 1        | 0.28          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 5        | 0.28          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 13       | 0.28          |
| (1,625)  | 1:111:A:GLY:H    | 1:109:A:ASP:HA   | 3        | 0.28          |
| (1,562)  | 1:43:A:ILE:H     | 1:43:A:ILE:HD11  | 1        | 0.28          |
| (1,562)  | 1:43:A:ILE:H     | 1:43:A:ILE:HD11  | 20       | 0.28          |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 7        | 0.28          |
| (1,95)   | 1:13:A:ILE:H     | 1:12:A:VAL:HG12  | 2        | 0.28          |
| (1,95)   | 1:13:A:ILE:H     | 1:12:A:VAL:HG12  | 9        | 0.28          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB2   | 13       | 0.28          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB3   | 18       | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (3,151)  | 1:104:A:LEU:HD22 | 1:18:A:LEU:HB3   | 19       | 0.27          |
| (3,9)    | 1:14:A:THR:H     | 1:111:A:GLY:HA2  | 17       | 0.27          |
| (1,1771) | 1:150:A:TYR:HA   | 1:154:A:ASN:HD22 | 3        | 0.27          |
| (1,1696) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HB   | 7        | 0.27          |
| (1,1696) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HB   | 10       | 0.27          |
| (1,1696) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HB   | 20       | 0.27          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 9        | 0.27          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 13       | 0.27          |
| (1,1654) | 1:133:A:ILE:HG21 | 1:5:A:TYR:HB2    | 19       | 0.27          |
| (1,1589) | 1:105:A:VAL:HG11 | 1:107:A:SER:H    | 3        | 0.27          |
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG21  | 7        | 0.27          |
| (1,1574) | 1:128:A:ILE:HD11 | 1:91:A:ILE:HD11  | 16       | 0.27          |
| (1,1574) | 1:128:A:ILE:HD11 | 1:91:A:ILE:HD13  | 20       | 0.27          |
| (1,1571) | 1:128:A:ILE:HD11 | 1:120:A:TYR:HA   | 11       | 0.27          |
| (1,1514) | 1:18:A:LEU:HD22  | 1:13:A:ILE:HA    | 6        | 0.27          |
| (1,1461) | 1:74:A:ILE:HG21  | 1:76:A:ASN:H     | 5        | 0.27          |
| (1,1461) | 1:74:A:ILE:HG23  | 1:76:A:ASN:H     | 9        | 0.27          |
| (1,1383) | 1:130:A:GLU:HG2  | 1:133:A:ILE:HG12 | 9        | 0.27          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 20       | 0.27          |
| (1,1335) | 1:128:A:ILE:HD11 | 1:128:A:ILE:HA   | 17       | 0.27          |
| (1,1289) | 1:52:A:THR:HB    | 1:71:A:ILE:HG23  | 6        | 0.27          |
| (1,1271) | 1:48:A:GLY:HA2   | 1:71:A:ILE:HG12  | 10       | 0.27          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 14       | 0.27          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 18       | 0.27          |
| (1,1141) | 1:102:A:ILE:HG23 | 1:116:A:SER:HB3  | 15       | 0.27          |
| (1,1134) | 1:30:A:ILE:HG23  | 1:37:A:ALA:HB2   | 10       | 0.27          |
| (1,1131) | 1:91:A:ILE:HG22  | 1:96:A:GLU:H     | 13       | 0.27          |
| (1,1111) | 1:30:A:ILE:HA    | 1:147:A:VAL:HG12 | 3        | 0.27          |
| (1,1111) | 1:30:A:ILE:HA    | 1:147:A:VAL:HG13 | 18       | 0.27          |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD11  | 4        | 0.27          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 16       | 0.27          |
| (1,994)  | 1:82:A:ALA:HB1   | 1:71:A:ILE:HA    | 5        | 0.27          |
| (1,976)  | 1:13:A:ILE:HG23  | 1:17:A:ARG:HB2   | 9        | 0.27          |
| (1,976)  | 1:13:A:ILE:HG22  | 1:17:A:ARG:HB2   | 11       | 0.27          |
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD1   | 6        | 0.27          |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG23  | 3        | 0.27          |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG21  | 11       | 0.27          |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG22  | 14       | 0.27          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 1        | 0.27          |
| (1,659)  | 1:115:A:LYS:H    | 1:115:A:LYS:HG2  | 10       | 0.27          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 14       | 0.27          |
| (1,625)  | 1:111:A:GLY:H    | 1:109:A:ASP:HA   | 19       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,519)  | 1:97:A:LYS:H     | 1:91:A:ILE:HD12  | 3        | 0.27          |
| (1,344)  | 1:64:A:PHE:H     | 1:57:A:THR:HG21  | 20       | 0.27          |
| (1,96)   | 1:146:A:ALA:H    | 1:145:A:LYS:HB2  | 1        | 0.27          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB3   | 17       | 0.27          |
| (3,179)  | 1:148:A:GLU:HA   | 1:152:A:LEU:HD21 | 8        | 0.26          |
| (3,172)  | 1:101:A:GLU:HA   | 1:81:A:TYR:H     | 1        | 0.26          |
| (3,172)  | 1:101:A:GLU:HA   | 1:81:A:TYR:H     | 6        | 0.26          |
| (3,172)  | 1:101:A:GLU:HA   | 1:81:A:TYR:H     | 9        | 0.26          |
| (3,151)  | 1:104:A:LEU:HD22 | 1:18:A:LEU:HB3   | 13       | 0.26          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 6        | 0.26          |
| (1,1696) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HB   | 1        | 0.26          |
| (1,1696) | 1:151:A:LEU:HD13 | 1:147:A:VAL:HB   | 17       | 0.26          |
| (1,1694) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HA   | 6        | 0.26          |
| (1,1661) | 1:143:A:ILE:HA   | 1:37:A:ALA:HB3   | 7        | 0.26          |
| (1,1618) | 1:114:A:LEU:HD21 | 1:9:A:THR:HB     | 8        | 0.26          |
| (1,1589) | 1:105:A:VAL:HG12 | 1:107:A:SER:H    | 2        | 0.26          |
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG21  | 19       | 0.26          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 5        | 0.26          |
| (1,1543) | 1:156:A:ALA:HB2  | 1:154:A:ASN:HA   | 11       | 0.26          |
| (1,1512) | 1:84:A:THR:HG21  | 1:71:A:ILE:HA    | 5        | 0.26          |
| (1,1512) | 1:84:A:THR:HG23  | 1:71:A:ILE:HA    | 12       | 0.26          |
| (1,1461) | 1:74:A:ILE:HG21  | 1:76:A:ASN:H     | 1        | 0.26          |
| (1,1461) | 1:74:A:ILE:HG22  | 1:76:A:ASN:H     | 3        | 0.26          |
| (1,1461) | 1:74:A:ILE:HG21  | 1:76:A:ASN:H     | 13       | 0.26          |
| (1,1461) | 1:74:A:ILE:HG22  | 1:76:A:ASN:H     | 14       | 0.26          |
| (1,1461) | 1:74:A:ILE:HG21  | 1:76:A:ASN:H     | 18       | 0.26          |
| (1,1461) | 1:74:A:ILE:HG22  | 1:76:A:ASN:H     | 19       | 0.26          |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD12  | 8        | 0.26          |
| (1,1367) | 1:58:A:PHE:HA    | 1:38:A:ILE:HD11  | 18       | 0.26          |
| (1,1335) | 1:128:A:ILE:HD11 | 1:128:A:ILE:HA   | 4        | 0.26          |
| (1,1326) | 1:85:A:LEU:HD23  | 1:85:A:LEU:HA    | 7        | 0.26          |
| (1,1245) | 1:44:A:ILE:HG21  | 1:44:A:ILE:HB    | 6        | 0.26          |
| (1,1245) | 1:44:A:ILE:HG23  | 1:44:A:ILE:HB    | 8        | 0.26          |
| (1,1245) | 1:44:A:ILE:HG22  | 1:44:A:ILE:HB    | 20       | 0.26          |
| (1,1204) | 1:38:A:ILE:HD12  | 1:58:A:PHE:HZ    | 19       | 0.26          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 1        | 0.26          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 6        | 0.26          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 7        | 0.26          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 11       | 0.26          |
| (1,1120) | 1:74:A:ILE:HD13  | 1:71:A:ILE:HA    | 11       | 0.26          |
| (1,1074) | 1:24:A:LEU:HA    | 1:43:A:ILE:HD11  | 20       | 0.26          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 7        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,995)  | 1:82:A:ALA:HB1   | 1:81:A:TYR:HB2   | 10       | 0.26          |
| (1,995)  | 1:82:A:ALA:HB3   | 1:81:A:TYR:HB2   | 14       | 0.26          |
| (1,994)  | 1:82:A:ALA:HB2   | 1:71:A:ILE:HA    | 20       | 0.26          |
| (1,940)  | 1:10:A:THR:HG22  | 1:107:A:SER:HB2  | 16       | 0.26          |
| (1,939)  | 1:80:A:THR:HG23  | 1:74:A:ILE:HA    | 20       | 0.26          |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG22  | 4        | 0.26          |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG22  | 8        | 0.26          |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3  | 11       | 0.26          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 12       | 0.26          |
| (1,720)  | 1:128:A:ILE:H    | 1:128:A:ILE:HG13 | 19       | 0.26          |
| (1,702)  | 1:122:A:THR:H    | 1:128:A:ILE:HG13 | 19       | 0.26          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD11  | 12       | 0.26          |
| (1,562)  | 1:43:A:ILE:H     | 1:43:A:ILE:HD11  | 3        | 0.26          |
| (1,562)  | 1:43:A:ILE:H     | 1:43:A:ILE:HD11  | 4        | 0.26          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 2        | 0.26          |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 13       | 0.26          |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 13       | 0.26          |
| (1,334)  | 1:59:A:GLY:H     | 1:58:A:PHE:HB2   | 3        | 0.26          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2   | 6        | 0.25          |
| (1,1696) | 1:151:A:LEU:HD13 | 1:147:A:VAL:HB   | 19       | 0.25          |
| (1,1661) | 1:143:A:ILE:HA   | 1:37:A:ALA:HB3   | 2        | 0.25          |
| (1,1661) | 1:143:A:ILE:HA   | 1:37:A:ALA:HB2   | 18       | 0.25          |
| (1,1654) | 1:133:A:ILE:HG23 | 1:5:A:TYR:HB2    | 6        | 0.25          |
| (1,1589) | 1:105:A:VAL:HG11 | 1:107:A:SER:H    | 14       | 0.25          |
| (1,1589) | 1:105:A:VAL:HG11 | 1:107:A:SER:H    | 15       | 0.25          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 11       | 0.25          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 13       | 0.25          |
| (1,1531) | 1:19:A:PHE:HB2   | 1:20:A:LYS:HG2   | 8        | 0.25          |
| (1,1461) | 1:74:A:ILE:HG21  | 1:76:A:ASN:H     | 6        | 0.25          |
| (1,1461) | 1:74:A:ILE:HG22  | 1:76:A:ASN:H     | 7        | 0.25          |
| (1,1461) | 1:74:A:ILE:HG22  | 1:76:A:ASN:H     | 10       | 0.25          |
| (1,1461) | 1:74:A:ILE:HG22  | 1:76:A:ASN:H     | 15       | 0.25          |
| (1,1245) | 1:44:A:ILE:HG21  | 1:44:A:ILE:HB    | 1        | 0.25          |
| (1,1245) | 1:44:A:ILE:HG21  | 1:44:A:ILE:HB    | 3        | 0.25          |
| (1,1245) | 1:44:A:ILE:HG22  | 1:44:A:ILE:HB    | 4        | 0.25          |
| (1,1245) | 1:44:A:ILE:HG22  | 1:44:A:ILE:HB    | 10       | 0.25          |
| (1,1245) | 1:44:A:ILE:HG21  | 1:44:A:ILE:HB    | 11       | 0.25          |
| (1,1245) | 1:44:A:ILE:HG21  | 1:44:A:ILE:HB    | 12       | 0.25          |
| (1,1245) | 1:44:A:ILE:HG22  | 1:44:A:ILE:HB    | 15       | 0.25          |
| (1,1146) | 1:31:A:PRO:HG2   | 1:41:A:SER:HB2   | 5        | 0.25          |
| (1,1141) | 1:102:A:ILE:HG22 | 1:116:A:SER:HB3  | 3        | 0.25          |
| (1,1141) | 1:102:A:ILE:HG23 | 1:116:A:SER:HB3  | 10       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1141) | 1:102:A:ILE:HG22 | 1:116:A:SER:HB3  | 11       | 0.25          |
| (1,1111) | 1:30:A:ILE:HA    | 1:147:A:VAL:HG12 | 7        | 0.25          |
| (1,1045) | 1:19:A:PHE:HB3   | 1:104:A:LEU:HD11 | 10       | 0.25          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 1        | 0.25          |
| (1,995)  | 1:82:A:ALA:HB3   | 1:81:A:TYR:HB2   | 3        | 0.25          |
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD1   | 4        | 0.25          |
| (1,921)  | 1:86:A:ILE:HA    | 1:86:A:ILE:HG21  | 17       | 0.25          |
| (1,888)  | 1:2:A:VAL:HG13   | 1:121:A:HIS:HA   | 14       | 0.25          |
| (1,840)  | 1:154:A:ASN:H    | 1:154:A:ASN:HB3  | 1        | 0.25          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 16       | 0.25          |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3  | 9        | 0.25          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 19       | 0.25          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 20       | 0.25          |
| (1,720)  | 1:128:A:ILE:H    | 1:128:A:ILE:HG13 | 3        | 0.25          |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD23  | 15       | 0.25          |
| (1,519)  | 1:97:A:LYS:H     | 1:91:A:ILE:HD12  | 4        | 0.25          |
| (1,364)  | 1:67:A:VAL:H     | 1:68:A:LYS:HG3   | 1        | 0.25          |
| (1,344)  | 1:64:A:PHE:H     | 1:57:A:THR:HG21  | 8        | 0.25          |
| (1,310)  | 1:56:A:ILE:H     | 1:67:A:VAL:HG11  | 5        | 0.25          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB2   | 9        | 0.25          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB3   | 16       | 0.25          |
| (1,71)   | 1:30:A:ILE:H     | 1:30:A:ILE:HG12  | 1        | 0.25          |
| (1,71)   | 1:30:A:ILE:H     | 1:30:A:ILE:HG12  | 11       | 0.25          |
| (1,71)   | 1:30:A:ILE:H     | 1:30:A:ILE:HG12  | 16       | 0.25          |
| (3,172)  | 1:101:A:GLU:HA   | 1:81:A:TYR:H     | 19       | 0.24          |
| (3,167)  | 1:146:A:ALA:HB1  | 1:35:A:PRO:HD2   | 14       | 0.24          |
| (3,103)  | 1:71:A:ILE:HG22  | 1:54:A:LYS:HE2   | 5        | 0.24          |
| (3,88)   | 1:151:A:LEU:HD22 | 1:17:A:ARG:HD3   | 18       | 0.24          |
| (1,1660) | 1:143:A:ILE:HA   | 1:144:A:PHE:HD2  | 14       | 0.24          |
| (1,1575) | 1:99:A:ALA:HA    | 1:84:A:THR:HG21  | 20       | 0.24          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 4        | 0.24          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 15       | 0.24          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 16       | 0.24          |
| (1,1551) | 1:114:A:LEU:HA   | 1:104:A:LEU:HD21 | 13       | 0.24          |
| (1,1429) | 1:104:A:LEU:HD12 | 1:106:A:ALA:H    | 5        | 0.24          |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD12  | 18       | 0.24          |
| (1,1300) | 1:71:A:ILE:HD11  | 1:70:A:ARG:HE    | 10       | 0.24          |
| (1,1271) | 1:48:A:GLY:HA2   | 1:71:A:ILE:HG12  | 19       | 0.24          |
| (1,1245) | 1:44:A:ILE:HG23  | 1:44:A:ILE:HB    | 13       | 0.24          |
| (1,1245) | 1:44:A:ILE:HG22  | 1:44:A:ILE:HB    | 18       | 0.24          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 12       | 0.24          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 3        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1127) | 1:71:A:ILE:HG23  | 1:82:A:ALA:HA    | 17       | 0.24          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 18       | 0.24          |
| (1,994)  | 1:82:A:ALA:HB2   | 1:71:A:ILE:HA    | 6        | 0.24          |
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD2   | 5        | 0.24          |
| (1,888)  | 1:2:A:VAL:HG13   | 1:121:A:HIS:HA   | 18       | 0.24          |
| (1,875)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:H    | 4        | 0.24          |
| (1,625)  | 1:111:A:GLY:H    | 1:109:A:ASP:HA   | 6        | 0.24          |
| (1,562)  | 1:43:A:ILE:H     | 1:43:A:ILE:HD11  | 6        | 0.24          |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 2        | 0.24          |
| (1,95)   | 1:13:A:ILE:H     | 1:12:A:VAL:HG13  | 10       | 0.24          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB1   | 7        | 0.24          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB1   | 14       | 0.24          |
| (1,71)   | 1:30:A:ILE:H     | 1:30:A:ILE:HG12  | 4        | 0.24          |
| (1,71)   | 1:30:A:ILE:H     | 1:30:A:ILE:HG12  | 10       | 0.24          |
| (1,71)   | 1:30:A:ILE:H     | 1:30:A:ILE:HG12  | 12       | 0.24          |
| (1,71)   | 1:30:A:ILE:H     | 1:30:A:ILE:HG12  | 13       | 0.24          |
| (3,172)  | 1:101:A:GLU:HA   | 1:100:A:TYR:H    | 16       | 0.23          |
| (3,171)  | 1:156:A:ALA:HA   | 1:159:A:HIS:HB2  | 2        | 0.23          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE2   | 11       | 0.23          |
| (3,32)   | 1:66:A:TYR:H     | 1:89:A:ASP:HB2   | 7        | 0.23          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 5        | 0.23          |
| (1,1571) | 1:128:A:ILE:HD12 | 1:120:A:TYR:HA   | 3        | 0.23          |
| (1,1551) | 1:114:A:LEU:HA   | 1:104:A:LEU:HD23 | 10       | 0.23          |
| (1,1512) | 1:84:A:THR:HG21  | 1:71:A:ILE:HA    | 11       | 0.23          |
| (1,1461) | 1:74:A:ILE:HG21  | 1:76:A:ASN:H     | 8        | 0.23          |
| (1,1461) | 1:74:A:ILE:HG22  | 1:76:A:ASN:H     | 16       | 0.23          |
| (1,1450) | 1:71:A:ILE:HG23  | 1:70:A:ARG:HE    | 15       | 0.23          |
| (1,1350) | 1:56:A:ILE:HG21  | 1:38:A:ILE:HG12  | 4        | 0.23          |
| (1,1346) | 1:56:A:ILE:HG22  | 1:58:A:PHE:HZ    | 5        | 0.23          |
| (1,1335) | 1:128:A:ILE:HD12 | 1:128:A:ILE:HA   | 6        | 0.23          |
| (1,1335) | 1:128:A:ILE:HD11 | 1:128:A:ILE:HA   | 16       | 0.23          |
| (1,1310) | 1:44:A:ILE:HD12  | 1:68:A:LYS:HD2   | 10       | 0.23          |
| (1,1281) | 1:155:A:PRO:HD3  | 1:151:A:LEU:HD21 | 16       | 0.23          |
| (1,1245) | 1:44:A:ILE:HG21  | 1:44:A:ILE:HB    | 5        | 0.23          |
| (1,1245) | 1:44:A:ILE:HG23  | 1:44:A:ILE:HB    | 19       | 0.23          |
| (1,1208) | 1:38:A:ILE:HG21  | 1:30:A:ILE:HB    | 15       | 0.23          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 5        | 0.23          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 19       | 0.23          |
| (1,1120) | 1:74:A:ILE:HD11  | 1:71:A:ILE:HA    | 8        | 0.23          |
| (1,1054) | 1:22:A:PHE:HA    | 1:29:A:LEU:HD12  | 14       | 0.23          |
| (1,1025) | 1:128:A:ILE:HA   | 1:129:A:LYS:H    | 20       | 0.23          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 5        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 6        | 0.23          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 9        | 0.23          |
| (1,995)  | 1:82:A:ALA:HB2   | 1:81:A:TYR:HB2   | 2        | 0.23          |
| (1,995)  | 1:82:A:ALA:HB2   | 1:81:A:TYR:HB2   | 16       | 0.23          |
| (1,976)  | 1:13:A:ILE:HG21  | 1:17:A:ARG:HB2   | 1        | 0.23          |
| (1,976)  | 1:13:A:ILE:HG23  | 1:17:A:ARG:HB2   | 16       | 0.23          |
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD2   | 7        | 0.23          |
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD2   | 12       | 0.23          |
| (1,940)  | 1:10:A:THR:HG23  | 1:107:A:SER:HB2  | 19       | 0.23          |
| (1,859)  | 1:78:A:ASN:HD21  | 1:77:A:ALA:HB3   | 6        | 0.23          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 3        | 0.23          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 9        | 0.23          |
| (1,535)  | 1:100:A:TYR:H    | 1:83:A:CYS:HB3   | 3        | 0.23          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 17       | 0.23          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 19       | 0.23          |
| (1,493)  | 1:90:A:ALA:H     | 1:67:A:VAL:HG11  | 8        | 0.23          |
| (1,479)  | 1:87:A:GLU:H     | 1:68:A:LYS:HB3   | 10       | 0.23          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB1   | 1        | 0.23          |
| (1,71)   | 1:30:A:ILE:H     | 1:30:A:ILE:HG12  | 18       | 0.23          |
| (1,47)   | 1:6:A:GLU:H      | 1:7:A:SER:HA     | 4        | 0.23          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2   | 2        | 0.22          |
| (3,172)  | 1:101:A:GLU:HA   | 1:100:A:TYR:H    | 4        | 0.22          |
| (3,172)  | 1:101:A:GLU:HA   | 1:100:A:TYR:H    | 18       | 0.22          |
| (3,167)  | 1:146:A:ALA:HB1  | 1:35:A:PRO:HD3   | 6        | 0.22          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 18       | 0.22          |
| (1,1762) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD22 | 14       | 0.22          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 16       | 0.22          |
| (1,1696) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HB   | 4        | 0.22          |
| (1,1696) | 1:151:A:LEU:HD12 | 1:147:A:VAL:HB   | 11       | 0.22          |
| (1,1660) | 1:143:A:ILE:HA   | 1:144:A:PHE:HD2  | 2        | 0.22          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 1        | 0.22          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 17       | 0.22          |
| (1,1551) | 1:114:A:LEU:HA   | 1:104:A:LEU:HD23 | 20       | 0.22          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 8        | 0.22          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 19       | 0.22          |
| (1,1310) | 1:44:A:ILE:HD11  | 1:68:A:LYS:HD2   | 16       | 0.22          |
| (1,1281) | 1:155:A:PRO:HD3  | 1:151:A:LEU:HD21 | 2        | 0.22          |
| (1,1245) | 1:44:A:ILE:HG23  | 1:44:A:ILE:HB    | 9        | 0.22          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 2        | 0.22          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 15       | 0.22          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 20       | 0.22          |
| (1,1152) | 1:151:A:LEU:HA   | 1:150:A:TYR:HB2  | 12       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1029) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD13 | 15       | 0.22          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 14       | 0.22          |
| (1,957)  | 1:11:A:THR:HG22  | 1:112:A:SER:HB2  | 16       | 0.22          |
| (1,940)  | 1:10:A:THR:HG21  | 1:107:A:SER:HB2  | 7        | 0.22          |
| (1,940)  | 1:10:A:THR:HG22  | 1:107:A:SER:HB2  | 12       | 0.22          |
| (1,890)  | 1:2:A:VAL:HG13   | 1:4:A:THR:HB     | 4        | 0.22          |
| (1,839)  | 1:154:A:ASN:H    | 1:153:A:ALA:HB3  | 2        | 0.22          |
| (1,839)  | 1:154:A:ASN:H    | 1:153:A:ALA:HB2  | 14       | 0.22          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 6        | 0.22          |
| (1,493)  | 1:90:A:ALA:H     | 1:67:A:VAL:HG11  | 19       | 0.22          |
| (1,477)  | 1:87:A:GLU:H     | 1:67:A:VAL:HG23  | 2        | 0.22          |
| (1,310)  | 1:56:A:ILE:H     | 1:67:A:VAL:HG13  | 14       | 0.22          |
| (1,233)  | 1:70:A:ARG:HH22  | 1:70:A:ARG:HB2   | 9        | 0.22          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB2   | 6        | 0.22          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB1   | 15       | 0.22          |
| (1,71)   | 1:30:A:ILE:H     | 1:30:A:ILE:HG12  | 6        | 0.22          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2   | 14       | 0.21          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2   | 19       | 0.21          |
| (3,172)  | 1:101:A:GLU:HA   | 1:81:A:TYR:H     | 12       | 0.21          |
| (3,153)  | 1:113:A:ILE:HD11 | 1:108:A:PRO:HG2  | 2        | 0.21          |
| (3,103)  | 1:71:A:ILE:HG23  | 1:54:A:LYS:HE2   | 20       | 0.21          |
| (3,9)    | 1:14:A:THR:H     | 1:111:A:GLY:HA2  | 10       | 0.21          |
| (3,9)    | 1:14:A:THR:H     | 1:111:A:GLY:HA2  | 16       | 0.21          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 11       | 0.21          |
| (1,1766) | 1:9:A:THR:HB     | 1:102:A:ILE:HG23 | 17       | 0.21          |
| (1,1765) | 1:2:A:VAL:HG13   | 1:3:A:PHE:HA     | 7        | 0.21          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 4        | 0.21          |
| (1,1699) | 1:153:A:ALA:HA   | 1:154:A:ASN:HA   | 13       | 0.21          |
| (1,1678) | 1:134:A:LYS:HA   | 1:134:A:LYS:HD3  | 10       | 0.21          |
| (1,1607) | 1:111:A:GLY:HA3  | 1:14:A:THR:HG21  | 4        | 0.21          |
| (1,1589) | 1:105:A:VAL:HG13 | 1:107:A:SER:H    | 17       | 0.21          |
| (1,1551) | 1:114:A:LEU:HA   | 1:104:A:LEU:HD22 | 7        | 0.21          |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 10       | 0.21          |
| (1,1336) | 1:128:A:ILE:HD13 | 1:120:A:TYR:HB2  | 5        | 0.21          |
| (1,1311) | 1:71:A:ILE:HD13  | 1:71:A:ILE:HG12  | 1        | 0.21          |
| (1,1311) | 1:71:A:ILE:HD13  | 1:71:A:ILE:HG12  | 7        | 0.21          |
| (1,1311) | 1:71:A:ILE:HD13  | 1:71:A:ILE:HG12  | 10       | 0.21          |
| (1,1311) | 1:71:A:ILE:HD13  | 1:71:A:ILE:HG12  | 15       | 0.21          |
| (1,1311) | 1:71:A:ILE:HD13  | 1:71:A:ILE:HG12  | 16       | 0.21          |
| (1,1311) | 1:71:A:ILE:HD12  | 1:71:A:ILE:HG12  | 20       | 0.21          |
| (1,1245) | 1:44:A:ILE:HG21  | 1:44:A:ILE:HB    | 16       | 0.21          |
| (1,1223) | 1:8:A:GLU:HG2    | 1:113:A:ILE:HG22 | 14       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 3        | 0.21          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 4        | 0.21          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 11       | 0.21          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 13       | 0.21          |
| (1,1168) | 1:33:A:VAL:HG11  | 1:150:A:TYR:HB3  | 12       | 0.21          |
| (1,1134) | 1:30:A:ILE:HG21  | 1:37:A:ALA:HB3   | 11       | 0.21          |
| (1,1111) | 1:30:A:ILE:HA    | 1:147:A:VAL:HG12 | 14       | 0.21          |
| (1,1091) | 1:27:A:ASP:HA    | 1:41:A:SER:HB2   | 18       | 0.21          |
| (1,1072) | 1:23:A:VAL:HG12  | 1:23:A:VAL:H     | 3        | 0.21          |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 10       | 0.21          |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 13       | 0.21          |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 20       | 0.21          |
| (1,1025) | 1:128:A:ILE:HA   | 1:129:A:LYS:H    | 15       | 0.21          |
| (1,995)  | 1:82:A:ALA:HB2   | 1:81:A:TYR:HB2   | 15       | 0.21          |
| (1,940)  | 1:10:A:THR:HG21  | 1:107:A:SER:HB2  | 2        | 0.21          |
| (1,940)  | 1:10:A:THR:HG23  | 1:107:A:SER:HB2  | 15       | 0.21          |
| (1,939)  | 1:80:A:THR:HG22  | 1:74:A:ILE:HA    | 12       | 0.21          |
| (1,939)  | 1:80:A:THR:HG23  | 1:74:A:ILE:HA    | 14       | 0.21          |
| (1,826)  | 1:153:A:ALA:H    | 1:151:A:LEU:HB3  | 3        | 0.21          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 6        | 0.21          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 11       | 0.21          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD12  | 15       | 0.21          |
| (1,657)  | 1:115:A:LYS:H    | 1:115:A:LYS:HB3  | 1        | 0.21          |
| (1,657)  | 1:115:A:LYS:H    | 1:115:A:LYS:HB3  | 5        | 0.21          |
| (1,657)  | 1:115:A:LYS:H    | 1:115:A:LYS:HB3  | 9        | 0.21          |
| (1,619)  | 1:110:A:GLY:H    | 1:109:A:ASP:HA   | 3        | 0.21          |
| (1,614)  | 1:110:A:GLY:H    | 1:106:A:ALA:HB2  | 17       | 0.21          |
| (1,603)  | 1:107:A:SER:H    | 1:107:A:SER:HB2  | 14       | 0.21          |
| (1,95)   | 1:13:A:ILE:H     | 1:12:A:VAL:HG12  | 19       | 0.21          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB2   | 4        | 0.21          |
| (1,71)   | 1:30:A:ILE:H     | 1:30:A:ILE:HG12  | 14       | 0.21          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB3   | 15       | 0.2           |
| (3,172)  | 1:101:A:GLU:HA   | 1:100:A:TYR:H    | 10       | 0.2           |
| (3,171)  | 1:156:A:ALA:HA   | 1:159:A:HIS:HB3  | 10       | 0.2           |
| (3,167)  | 1:146:A:ALA:HB3  | 1:35:A:PRO:HD2   | 18       | 0.2           |
| (3,147)  | 1:80:A:THR:HA    | 1:103:A:LYS:HD2  | 8        | 0.2           |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 8        | 0.2           |
| (1,1762) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD22 | 1        | 0.2           |
| (1,1696) | 1:151:A:LEU:HD13 | 1:147:A:VAL:HB   | 18       | 0.2           |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 7        | 0.2           |
| (1,1574) | 1:128:A:ILE:HD11 | 1:91:A:ILE:HD12  | 3        | 0.2           |
| (1,1574) | 1:128:A:ILE:HD12 | 1:91:A:ILE:HD12  | 10       | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1574) | 1:128:A:ILE:HD11 | 1:91:A:ILE:HD11  | 19       | 0.2           |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2  | 11       | 0.2           |
| (1,1557) | 1:85:A:LEU:HD13  | 1:91:A:ILE:HG12  | 20       | 0.2           |
| (1,1550) | 1:114:A:LEU:HA   | 1:115:A:LYS:HB3  | 18       | 0.2           |
| (1,1530) | 1:45:A:GLU:HA    | 1:43:A:ILE:HG23  | 3        | 0.2           |
| (1,1503) | 1:117:A:THR:HA   | 1:6:A:GLU:HB3    | 9        | 0.2           |
| (1,1456) | 1:127:A:GLU:HG3  | 1:127:A:GLU:H    | 2        | 0.2           |
| (1,1351) | 1:56:A:ILE:HG21  | 1:38:A:ILE:HG21  | 20       | 0.2           |
| (1,1350) | 1:56:A:ILE:HG21  | 1:38:A:ILE:HG12  | 15       | 0.2           |
| (1,1311) | 1:71:A:ILE:HD12  | 1:71:A:ILE:HG12  | 2        | 0.2           |
| (1,1311) | 1:71:A:ILE:HD11  | 1:71:A:ILE:HG12  | 12       | 0.2           |
| (1,1311) | 1:71:A:ILE:HD12  | 1:71:A:ILE:HG12  | 17       | 0.2           |
| (1,1311) | 1:71:A:ILE:HD11  | 1:71:A:ILE:HG12  | 18       | 0.2           |
| (1,1311) | 1:71:A:ILE:HD11  | 1:71:A:ILE:HG12  | 19       | 0.2           |
| (1,1245) | 1:44:A:ILE:HG21  | 1:44:A:ILE:HB    | 17       | 0.2           |
| (1,1243) | 1:53:A:ILE:HG12  | 1:45:A:GLU:HG3   | 9        | 0.2           |
| (1,1232) | 1:133:A:ILE:HG13 | 1:132:A:GLN:HB2  | 19       | 0.2           |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 6        | 0.2           |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 10       | 0.2           |
| (1,1166) | 1:33:A:VAL:HG13  | 1:29:A:LEU:H     | 1        | 0.2           |
| (1,1146) | 1:31:A:PRO:HG2   | 1:41:A:SER:HB2   | 18       | 0.2           |
| (1,1129) | 1:30:A:ILE:HG22  | 1:37:A:ALA:H     | 5        | 0.2           |
| (1,1127) | 1:71:A:ILE:HG22  | 1:82:A:ALA:HA    | 7        | 0.2           |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 2        | 0.2           |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 7        | 0.2           |
| (1,1029) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD13 | 2        | 0.2           |
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD2   | 1        | 0.2           |
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD1   | 11       | 0.2           |
| (1,839)  | 1:154:A:ASN:H    | 1:153:A:ALA:HB1  | 13       | 0.2           |
| (1,839)  | 1:154:A:ASN:H    | 1:153:A:ALA:HB1  | 20       | 0.2           |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 15       | 0.2           |
| (1,702)  | 1:122:A:THR:H    | 1:128:A:ILE:HG13 | 18       | 0.2           |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD13  | 2        | 0.2           |
| (1,657)  | 1:115:A:LYS:H    | 1:115:A:LYS:HB3  | 7        | 0.2           |
| (1,657)  | 1:115:A:LYS:H    | 1:115:A:LYS:HB3  | 13       | 0.2           |
| (1,657)  | 1:115:A:LYS:H    | 1:115:A:LYS:HB3  | 16       | 0.2           |
| (1,657)  | 1:115:A:LYS:H    | 1:115:A:LYS:HB3  | 17       | 0.2           |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 4        | 0.2           |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 19       | 0.2           |
| (1,619)  | 1:110:A:GLY:H    | 1:109:A:ASP:HA   | 4        | 0.2           |
| (1,527)  | 1:99:A:ALA:H     | 1:85:A:LEU:HD21  | 4        | 0.2           |
| (1,519)  | 1:97:A:LYS:H     | 1:91:A:ILE:HD12  | 17       | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,507)  | 1:96:A:GLU:H     | 1:95:A:LEU:HB2   | 6        | 0.2           |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 10       | 0.2           |
| (1,310)  | 1:56:A:ILE:H     | 1:67:A:VAL:HG12  | 4        | 0.2           |
| (1,137)  | 1:20:A:LYS:H     | 1:16:A:ALA:HB3   | 12       | 0.2           |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB2   | 2        | 0.2           |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB3   | 20       | 0.2           |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2    | 20       | 0.19          |
| (3,37)   | 1:82:A:ALA:H     | 1:19:A:PHE:HE2   | 4        | 0.19          |
| (1,1765) | 1:2:A:VAL:HG11   | 1:3:A:PHE:HA     | 2        | 0.19          |
| (1,1678) | 1:134:A:LYS:HA   | 1:134:A:LYS:HD3  | 17       | 0.19          |
| (1,1654) | 1:133:A:ILE:HG23 | 1:5:A:TYR:HB2    | 5        | 0.19          |
| (1,1654) | 1:133:A:ILE:HG23 | 1:5:A:TYR:HB2    | 16       | 0.19          |
| (1,1631) | 1:122:A:THR:HA   | 1:122:A:THR:HG23 | 2        | 0.19          |
| (1,1626) | 1:118:A:SER:HB2  | 1:117:A:THR:HG21 | 13       | 0.19          |
| (1,1551) | 1:114:A:LEU:HA   | 1:104:A:LEU:HD21 | 19       | 0.19          |
| (1,1541) | 1:143:A:ILE:HA   | 1:30:A:ILE:HG12  | 12       | 0.19          |
| (1,1512) | 1:84:A:THR:HG23  | 1:71:A:ILE:HA    | 1        | 0.19          |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD11  | 16       | 0.19          |
| (1,1351) | 1:56:A:ILE:HG21  | 1:38:A:ILE:HG23  | 15       | 0.19          |
| (1,1311) | 1:71:A:ILE:HD12  | 1:71:A:ILE:HG12  | 3        | 0.19          |
| (1,1311) | 1:71:A:ILE:HD11  | 1:71:A:ILE:HG12  | 4        | 0.19          |
| (1,1311) | 1:71:A:ILE:HD11  | 1:71:A:ILE:HG12  | 8        | 0.19          |
| (1,1311) | 1:71:A:ILE:HD13  | 1:71:A:ILE:HG12  | 9        | 0.19          |
| (1,1311) | 1:71:A:ILE:HD13  | 1:71:A:ILE:HG12  | 11       | 0.19          |
| (1,1300) | 1:71:A:ILE:HD13  | 1:70:A:ARG:HE    | 9        | 0.19          |
| (1,1300) | 1:71:A:ILE:HD11  | 1:70:A:ARG:HE    | 18       | 0.19          |
| (1,1245) | 1:44:A:ILE:HG22  | 1:44:A:ILE:HB    | 2        | 0.19          |
| (1,1245) | 1:44:A:ILE:HG21  | 1:44:A:ILE:HB    | 7        | 0.19          |
| (1,1232) | 1:133:A:ILE:HG13 | 1:132:A:GLN:HB2  | 3        | 0.19          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG22  | 17       | 0.19          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 9        | 0.19          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 18       | 0.19          |
| (1,1168) | 1:33:A:VAL:HG13  | 1:150:A:TYR:HB3  | 3        | 0.19          |
| (1,1168) | 1:33:A:VAL:HG11  | 1:150:A:TYR:HB3  | 8        | 0.19          |
| (1,1072) | 1:23:A:VAL:HG13  | 1:23:A:VAL:H     | 1        | 0.19          |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 17       | 0.19          |
| (1,1021) | 1:128:A:ILE:HA   | 1:127:A:GLU:HB2  | 13       | 0.19          |
| (1,997)  | 1:82:A:ALA:HB2   | 1:73:A:GLU:HB3   | 7        | 0.19          |
| (1,939)  | 1:80:A:THR:HG21  | 1:74:A:ILE:HA    | 9        | 0.19          |
| (1,859)  | 1:78:A:ASN:HD21  | 1:77:A:ALA:HB3   | 13       | 0.19          |
| (1,823)  | 1:153:A:ALA:H    | 1:17:A:ARG:HH11  | 10       | 0.19          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 4        | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,772)  | 1:141:A:SER:H    | 1:141:A:SER:HB3  | 3        | 0.19          |
| (1,771)  | 1:139:A:GLU:H    | 1:136:A:GLY:H    | 12       | 0.19          |
| (1,771)  | 1:139:A:GLU:H    | 1:136:A:GLY:H    | 19       | 0.19          |
| (1,700)  | 1:121:A:HIS:H    | 1:85:A:LEU:HD13  | 8        | 0.19          |
| (1,657)  | 1:115:A:LYS:H    | 1:115:A:LYS:HB3  | 2        | 0.19          |
| (1,657)  | 1:115:A:LYS:H    | 1:115:A:LYS:HB3  | 3        | 0.19          |
| (1,657)  | 1:115:A:LYS:H    | 1:115:A:LYS:HB3  | 14       | 0.19          |
| (1,657)  | 1:115:A:LYS:H    | 1:115:A:LYS:HB3  | 18       | 0.19          |
| (1,648)  | 1:114:A:LEU:H    | 1:113:A:ILE:HG21 | 10       | 0.19          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 1        | 0.19          |
| (1,619)  | 1:110:A:GLY:H    | 1:109:A:ASP:HA   | 19       | 0.19          |
| (1,540)  | 1:101:A:GLU:H    | 1:116:A:SER:HA   | 18       | 0.19          |
| (1,519)  | 1:97:A:LYS:H     | 1:91:A:ILE:HD12  | 1        | 0.19          |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 7        | 0.19          |
| (1,397)  | 1:75:A:ASP:H     | 1:73:A:GLU:HG3   | 9        | 0.19          |
| (1,373)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB3   | 7        | 0.19          |
| (1,373)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB3   | 12       | 0.19          |
| (1,347)  | 1:66:A:TYR:H     | 1:65:A:ASN:HB2   | 6        | 0.19          |
| (1,344)  | 1:64:A:PHE:H     | 1:57:A:THR:HG23  | 19       | 0.19          |
| (1,343)  | 1:63:A:GLN:HE22  | 1:63:A:GLN:HA    | 15       | 0.19          |
| (1,195)  | 1:36:A:GLN:H     | 1:36:A:GLN:HB2   | 6        | 0.19          |
| (1,128)  | 1:18:A:LEU:H     | 1:13:A:ILE:HG23  | 2        | 0.19          |
| (1,93)   | 1:143:A:ILE:H    | 1:34:A:ALA:HB2   | 11       | 0.19          |
| (1,47)   | 1:6:A:GLU:H      | 1:7:A:SER:HA     | 18       | 0.19          |
| (4,33)   | 1:87:A:GLU:H     | 1:68:A:LYS:O     | 6        | 0.18          |
| (4,33)   | 1:87:A:GLU:H     | 1:68:A:LYS:O     | 20       | 0.18          |
| (3,172)  | 1:101:A:GLU:HA   | 1:100:A:TYR:H    | 14       | 0.18          |
| (3,171)  | 1:156:A:ALA:HA   | 1:159:A:HIS:HB2  | 16       | 0.18          |
| (3,167)  | 1:146:A:ALA:HB3  | 1:35:A:PRO:HD2   | 19       | 0.18          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 17       | 0.18          |
| (1,1762) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD21 | 4        | 0.18          |
| (1,1762) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD23 | 7        | 0.18          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 2        | 0.18          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 9        | 0.18          |
| (1,1678) | 1:134:A:LYS:HA   | 1:134:A:LYS:HD3  | 3        | 0.18          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 18       | 0.18          |
| (1,1559) | 1:96:A:GLU:HA    | 1:91:A:ILE:HD12  | 12       | 0.18          |
| (1,1551) | 1:114:A:LEU:HA   | 1:104:A:LEU:HD21 | 11       | 0.18          |
| (1,1337) | 1:113:A:ILE:HD11 | 1:10:A:THR:HG22  | 10       | 0.18          |
| (1,1311) | 1:71:A:ILE:HD12  | 1:71:A:ILE:HG12  | 5        | 0.18          |
| (1,1311) | 1:71:A:ILE:HD13  | 1:71:A:ILE:HG12  | 6        | 0.18          |
| (1,1300) | 1:71:A:ILE:HD12  | 1:70:A:ARG:HE    | 2        | 0.18          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1289) | 1:52:A:THR:HB   | 1:71:A:ILE:HG22  | 8        | 0.18          |
| (1,1281) | 1:155:A:PRO:HD3 | 1:151:A:LEU:HD23 | 12       | 0.18          |
| (1,1211) | 1:38:A:ILE:HG23 | 1:38:A:ILE:HG12  | 7        | 0.18          |
| (1,1198) | 1:53:A:ILE:HB   | 1:53:A:ILE:HG22  | 3        | 0.18          |
| (1,1198) | 1:53:A:ILE:HB   | 1:53:A:ILE:HG22  | 5        | 0.18          |
| (1,1198) | 1:53:A:ILE:HB   | 1:53:A:ILE:HG21  | 7        | 0.18          |
| (1,1198) | 1:53:A:ILE:HB   | 1:53:A:ILE:HG21  | 16       | 0.18          |
| (1,1183) | 1:34:A:ALA:HB1  | 1:147:A:VAL:HG11 | 4        | 0.18          |
| (1,1176) | 1:34:A:ALA:HA   | 1:30:A:ILE:HA    | 16       | 0.18          |
| (1,1166) | 1:33:A:VAL:HG12 | 1:29:A:LEU:H     | 8        | 0.18          |
| (1,1051) | 1:148:A:GLU:HB3 | 1:144:A:PHE:HB3  | 12       | 0.18          |
| (1,1051) | 1:148:A:GLU:HB3 | 1:144:A:PHE:HB3  | 19       | 0.18          |
| (1,1029) | 1:17:A:ARG:HB3  | 1:151:A:LEU:HD13 | 10       | 0.18          |
| (1,997)  | 1:82:A:ALA:HB1  | 1:73:A:GLU:HB3   | 16       | 0.18          |
| (1,994)  | 1:82:A:ALA:HB2  | 1:71:A:ILE:HA    | 7        | 0.18          |
| (1,994)  | 1:82:A:ALA:HB2  | 1:71:A:ILE:HA    | 18       | 0.18          |
| (1,957)  | 1:11:A:THR:HG23 | 1:112:A:SER:HB2  | 10       | 0.18          |
| (1,950)  | 1:11:A:THR:HB   | 1:22:A:PHE:HD1   | 14       | 0.18          |
| (1,950)  | 1:11:A:THR:HB   | 1:22:A:PHE:HD1   | 16       | 0.18          |
| (1,839)  | 1:154:A:ASN:H   | 1:153:A:ALA:HB1  | 9        | 0.18          |
| (1,772)  | 1:141:A:SER:H   | 1:141:A:SER:HB3  | 1        | 0.18          |
| (1,772)  | 1:141:A:SER:H   | 1:141:A:SER:HB3  | 5        | 0.18          |
| (1,772)  | 1:141:A:SER:H   | 1:141:A:SER:HB3  | 6        | 0.18          |
| (1,772)  | 1:141:A:SER:H   | 1:141:A:SER:HB3  | 7        | 0.18          |
| (1,771)  | 1:139:A:GLU:H   | 1:136:A:GLY:H    | 20       | 0.18          |
| (1,702)  | 1:122:A:THR:H   | 1:128:A:ILE:HG13 | 8        | 0.18          |
| (1,700)  | 1:121:A:HIS:H   | 1:85:A:LEU:HD11  | 17       | 0.18          |
| (1,657)  | 1:115:A:LYS:H   | 1:115:A:LYS:HB3  | 4        | 0.18          |
| (1,657)  | 1:115:A:LYS:H   | 1:115:A:LYS:HB3  | 8        | 0.18          |
| (1,657)  | 1:115:A:LYS:H   | 1:115:A:LYS:HB3  | 11       | 0.18          |
| (1,657)  | 1:115:A:LYS:H   | 1:115:A:LYS:HB3  | 12       | 0.18          |
| (1,657)  | 1:115:A:LYS:H   | 1:115:A:LYS:HB3  | 15       | 0.18          |
| (1,520)  | 1:97:A:LYS:H    | 1:121:A:HIS:HB3  | 11       | 0.18          |
| (1,519)  | 1:97:A:LYS:H    | 1:91:A:ILE:HD13  | 8        | 0.18          |
| (1,494)  | 1:91:A:ILE:H    | 1:91:A:ILE:HG13  | 5        | 0.18          |
| (1,364)  | 1:67:A:VAL:H    | 1:68:A:LYS:HG3   | 3        | 0.18          |
| (1,292)  | 1:52:A:THR:H    | 1:46:A:GLY:HA2   | 16       | 0.18          |
| (1,233)  | 1:70:A:ARG:HH22 | 1:70:A:ARG:HB2   | 8        | 0.18          |
| (1,93)   | 1:143:A:ILE:H   | 1:34:A:ALA:HB3   | 19       | 0.18          |
| (3,167)  | 1:146:A:ALA:HB2 | 1:35:A:PRO:HD3   | 2        | 0.17          |
| (3,158)  | 1:118:A:SER:HB2 | 1:6:A:GLU:HG2    | 19       | 0.17          |
| (1,1781) | 1:157:A:ALA:HA  | 1:158:A:TYR:HA   | 3        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 13       | 0.17          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 14       | 0.17          |
| (1,1762) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD21 | 20       | 0.17          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 8        | 0.17          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 11       | 0.17          |
| (1,1697) | 1:151:A:LEU:HD11 | 1:150:A:TYR:HD1  | 1        | 0.17          |
| (1,1660) | 1:143:A:ILE:HA   | 1:144:A:PHE:HD2  | 13       | 0.17          |
| (1,1656) | 1:135:A:ALA:HA   | 1:139:A:GLU:HB2  | 12       | 0.17          |
| (1,1631) | 1:122:A:THR:HA   | 1:122:A:THR:HG21 | 5        | 0.17          |
| (1,1626) | 1:118:A:SER:HB2  | 1:117:A:THR:HG23 | 12       | 0.17          |
| (1,1626) | 1:118:A:SER:HB2  | 1:117:A:THR:HG23 | 18       | 0.17          |
| (1,1541) | 1:143:A:ILE:HA   | 1:30:A:ILE:HG12  | 14       | 0.17          |
| (1,1432) | 1:69:A:HIS:HA    | 1:69:A:HIS:HD2   | 14       | 0.17          |
| (1,1340) | 1:128:A:ILE:HD13 | 1:98:A:ILE:HG23  | 11       | 0.17          |
| (1,1340) | 1:128:A:ILE:HD11 | 1:98:A:ILE:HG21  | 20       | 0.17          |
| (1,1311) | 1:71:A:ILE:HD12  | 1:71:A:ILE:HG12  | 13       | 0.17          |
| (1,1311) | 1:71:A:ILE:HD13  | 1:71:A:ILE:HG12  | 14       | 0.17          |
| (1,1300) | 1:71:A:ILE:HD11  | 1:70:A:ARG:HE    | 8        | 0.17          |
| (1,1245) | 1:44:A:ILE:HG23  | 1:44:A:ILE:HB    | 14       | 0.17          |
| (1,1234) | 1:133:A:ILE:HG13 | 1:128:A:ILE:HG22 | 12       | 0.17          |
| (1,1232) | 1:133:A:ILE:HG13 | 1:132:A:GLN:HB2  | 13       | 0.17          |
| (1,1211) | 1:38:A:ILE:HG21  | 1:38:A:ILE:HG12  | 3        | 0.17          |
| (1,1211) | 1:38:A:ILE:HG23  | 1:38:A:ILE:HG12  | 12       | 0.17          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG21  | 4        | 0.17          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG22  | 10       | 0.17          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG21  | 12       | 0.17          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG22  | 14       | 0.17          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG21  | 18       | 0.17          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG23  | 19       | 0.17          |
| (1,1183) | 1:34:A:ALA:HB1   | 1:147:A:VAL:HG11 | 3        | 0.17          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 17       | 0.17          |
| (1,1091) | 1:27:A:ASP:HA    | 1:41:A:SER:HB2   | 5        | 0.17          |
| (1,1072) | 1:23:A:VAL:HG12  | 1:23:A:VAL:H     | 6        | 0.17          |
| (1,1072) | 1:23:A:VAL:HG12  | 1:23:A:VAL:H     | 19       | 0.17          |
| (1,1072) | 1:23:A:VAL:HG12  | 1:23:A:VAL:H     | 20       | 0.17          |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 6        | 0.17          |
| (1,1051) | 1:148:A:GLU:HB3  | 1:144:A:PHE:HB3  | 8        | 0.17          |
| (1,1029) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD11 | 8        | 0.17          |
| (1,995)  | 1:82:A:ALA:HB3   | 1:81:A:TYR:HB2   | 7        | 0.17          |
| (1,957)  | 1:11:A:THR:HG21  | 1:112:A:SER:HB2  | 11       | 0.17          |
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD2   | 13       | 0.17          |
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD1   | 19       | 0.17          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD2  | 20       | 0.17          |
| (1,940)  | 1:10:A:THR:HG23  | 1:107:A:SER:HB2 | 6        | 0.17          |
| (1,940)  | 1:10:A:THR:HG21  | 1:107:A:SER:HB2 | 8        | 0.17          |
| (1,940)  | 1:10:A:THR:HG22  | 1:107:A:SER:HB2 | 11       | 0.17          |
| (1,940)  | 1:10:A:THR:HG21  | 1:107:A:SER:HB2 | 13       | 0.17          |
| (1,940)  | 1:10:A:THR:HG21  | 1:107:A:SER:HB2 | 17       | 0.17          |
| (1,940)  | 1:10:A:THR:HG21  | 1:107:A:SER:HB2 | 18       | 0.17          |
| (1,875)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:H   | 14       | 0.17          |
| (1,833)  | 1:154:A:ASN:H    | 1:17:A:ARG:HH11 | 13       | 0.17          |
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3 | 10       | 0.17          |
| (1,772)  | 1:141:A:SER:H    | 1:141:A:SER:HB3 | 2        | 0.17          |
| (1,772)  | 1:141:A:SER:H    | 1:141:A:SER:HB3 | 14       | 0.17          |
| (1,772)  | 1:141:A:SER:H    | 1:141:A:SER:HB3 | 16       | 0.17          |
| (1,772)  | 1:141:A:SER:H    | 1:141:A:SER:HB3 | 20       | 0.17          |
| (1,771)  | 1:139:A:GLU:H    | 1:136:A:GLY:H   | 4        | 0.17          |
| (1,771)  | 1:139:A:GLU:H    | 1:136:A:GLY:H   | 18       | 0.17          |
| (1,708)  | 1:122:A:THR:H    | 1:95:A:LEU:HA   | 7        | 0.17          |
| (1,619)  | 1:110:A:GLY:H    | 1:109:A:ASP:HA  | 14       | 0.17          |
| (1,540)  | 1:101:A:GLU:H    | 1:116:A:SER:HA  | 3        | 0.17          |
| (1,540)  | 1:101:A:GLU:H    | 1:116:A:SER:HA  | 14       | 0.17          |
| (1,479)  | 1:87:A:GLU:H     | 1:68:A:LYS:HB3  | 2        | 0.17          |
| (1,404)  | 1:75:A:ASP:H     | 1:81:A:TYR:H    | 9        | 0.17          |
| (1,373)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB3  | 10       | 0.17          |
| (1,373)  | 1:70:A:ARG:H     | 1:69:A:HIS:HB3  | 20       | 0.17          |
| (1,347)  | 1:66:A:TYR:H     | 1:65:A:ASN:HB2  | 9        | 0.17          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2  | 17       | 0.17          |
| (1,195)  | 1:36:A:GLN:H     | 1:36:A:GLN:HB2  | 12       | 0.17          |
| (1,195)  | 1:36:A:GLN:H     | 1:36:A:GLN:HB2  | 16       | 0.17          |
| (1,95)   | 1:13:A:ILE:H     | 1:12:A:VAL:HG12 | 8        | 0.17          |
| (1,47)   | 1:6:A:GLU:H      | 1:7:A:SER:HA    | 3        | 0.17          |
| (4,33)   | 1:87:A:GLU:H     | 1:68:A:LYS:O    | 7        | 0.16          |
| (4,33)   | 1:87:A:GLU:H     | 1:68:A:LYS:O    | 19       | 0.16          |
| (4,27)   | 1:66:A:TYR:H     | 1:89:A:ASP:O    | 7        | 0.16          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2  | 13       | 0.16          |
| (3,151)  | 1:104:A:LEU:HD21 | 1:114:A:LEU:HG  | 6        | 0.16          |
| (3,149)  | 1:4:A:THR:HG22   | 1:6:A:GLU:HB2   | 8        | 0.16          |
| (3,46)   | 1:103:A:LYS:H    | 1:101:A:GLU:HB3 | 1        | 0.16          |
| (3,23)   | 1:45:A:GLU:H     | 1:53:A:ILE:HG22 | 14       | 0.16          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA  | 4        | 0.16          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA  | 8        | 0.16          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA  | 9        | 0.16          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA  | 10       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 18       | 0.16          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 20       | 0.16          |
| (1,1660) | 1:143:A:ILE:HA   | 1:144:A:PHE:HD1  | 18       | 0.16          |
| (1,1631) | 1:122:A:THR:HA   | 1:122:A:THR:HG22 | 20       | 0.16          |
| (1,1574) | 1:128:A:ILE:HD11 | 1:91:A:ILE:HD12  | 4        | 0.16          |
| (1,1574) | 1:128:A:ILE:HD13 | 1:91:A:ILE:HD12  | 12       | 0.16          |
| (1,1574) | 1:128:A:ILE:HD11 | 1:91:A:ILE:HD12  | 17       | 0.16          |
| (1,1531) | 1:19:A:PHE:HB2   | 1:20:A:LYS:HG2   | 18       | 0.16          |
| (1,1461) | 1:74:A:ILE:HG22  | 1:76:A:ASN:H     | 17       | 0.16          |
| (1,1429) | 1:104:A:LEU:HD13 | 1:106:A:ALA:H    | 9        | 0.16          |
| (1,1351) | 1:56:A:ILE:HG22  | 1:38:A:ILE:HG21  | 11       | 0.16          |
| (1,1351) | 1:56:A:ILE:HG23  | 1:38:A:ILE:HG21  | 17       | 0.16          |
| (1,1337) | 1:113:A:ILE:HD12 | 1:10:A:THR:HG22  | 11       | 0.16          |
| (1,1312) | 1:44:A:ILE:HG12  | 1:55:A:LYS:HE3   | 19       | 0.16          |
| (1,1300) | 1:71:A:ILE:HD12  | 1:70:A:ARG:HE    | 17       | 0.16          |
| (1,1272) | 1:136:A:GLY:HA3  | 1:139:A:GLU:HB3  | 19       | 0.16          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG21  | 1        | 0.16          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG23  | 2        | 0.16          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG21  | 6        | 0.16          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG21  | 8        | 0.16          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG21  | 15       | 0.16          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG21  | 20       | 0.16          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 1        | 0.16          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 14       | 0.16          |
| (1,1168) | 1:33:A:VAL:HG12  | 1:150:A:TYR:HB3  | 9        | 0.16          |
| (1,1133) | 1:91:A:ILE:HG21  | 1:95:A:LEU:HB3   | 11       | 0.16          |
| (1,1133) | 1:91:A:ILE:HG22  | 1:95:A:LEU:HB3   | 14       | 0.16          |
| (1,1111) | 1:30:A:ILE:HA    | 1:147:A:VAL:HG12 | 15       | 0.16          |
| (1,1064) | 1:41:A:SER:HB3   | 1:56:A:ILE:HA    | 15       | 0.16          |
| (1,1054) | 1:22:A:PHE:HA    | 1:29:A:LEU:HD13  | 7        | 0.16          |
| (1,1047) | 1:20:A:LYS:HA    | 1:23:A:VAL:HB    | 8        | 0.16          |
| (1,1047) | 1:20:A:LYS:HA    | 1:23:A:VAL:HB    | 17       | 0.16          |
| (1,1029) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD11 | 12       | 0.16          |
| (1,1025) | 1:128:A:ILE:HA   | 1:129:A:LYS:H    | 12       | 0.16          |
| (1,995)  | 1:82:A:ALA:HB2   | 1:81:A:TYR:HB2   | 6        | 0.16          |
| (1,994)  | 1:82:A:ALA:HB2   | 1:71:A:ILE:HA    | 13       | 0.16          |
| (1,943)  | 1:117:A:THR:HG21 | 1:101:A:GLU:HB3  | 4        | 0.16          |
| (1,940)  | 1:10:A:THR:HG22  | 1:107:A:SER:HB2  | 9        | 0.16          |
| (1,940)  | 1:10:A:THR:HG23  | 1:107:A:SER:HB2  | 20       | 0.16          |
| (1,875)  | 1:154:A:ASN:HD22 | 1:154:A:ASN:H    | 9        | 0.16          |
| (1,859)  | 1:78:A:ASN:HD21  | 1:77:A:ALA:HB3   | 3        | 0.16          |
| (1,837)  | 1:154:A:ASN:H    | 1:149:A:ALA:HA   | 16       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,795)  | 1:146:A:ALA:H    | 1:142:A:GLY:HA3  | 8        | 0.16          |
| (1,793)  | 1:146:A:ALA:H    | 1:143:A:ILE:HB   | 13       | 0.16          |
| (1,772)  | 1:141:A:SER:H    | 1:141:A:SER:HB3  | 15       | 0.16          |
| (1,772)  | 1:141:A:SER:H    | 1:141:A:SER:HB3  | 19       | 0.16          |
| (1,771)  | 1:139:A:GLU:H    | 1:136:A:GLY:H    | 10       | 0.16          |
| (1,708)  | 1:122:A:THR:H    | 1:95:A:LEU:HA    | 12       | 0.16          |
| (1,640)  | 1:113:A:ILE:H    | 1:114:A:LEU:HG   | 2        | 0.16          |
| (1,640)  | 1:113:A:ILE:H    | 1:114:A:LEU:HG   | 15       | 0.16          |
| (1,640)  | 1:113:A:ILE:H    | 1:114:A:LEU:HG   | 17       | 0.16          |
| (1,619)  | 1:110:A:GLY:H    | 1:109:A:ASP:HA   | 13       | 0.16          |
| (1,540)  | 1:101:A:GLU:H    | 1:116:A:SER:HA   | 4        | 0.16          |
| (1,540)  | 1:101:A:GLU:H    | 1:116:A:SER:HA   | 6        | 0.16          |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 8        | 0.16          |
| (1,375)  | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 18       | 0.16          |
| (1,334)  | 1:59:A:GLY:H     | 1:58:A:PHE:HB2   | 7        | 0.16          |
| (1,254)  | 1:45:A:GLU:H     | 1:53:A:ILE:HG12  | 3        | 0.16          |
| (1,233)  | 1:70:A:ARG:HH22  | 1:70:A:ARG:HB2   | 12       | 0.16          |
| (1,162)  | 1:24:A:LEU:H     | 1:20:A:LYS:HB3   | 19       | 0.16          |
| (1,71)   | 1:30:A:ILE:H     | 1:30:A:ILE:HG12  | 20       | 0.16          |
| (1,47)   | 1:6:A:GLU:H      | 1:7:A:SER:HA     | 5        | 0.16          |
| (4,33)   | 1:87:A:GLU:H     | 1:68:A:LYS:O     | 1        | 0.15          |
| (3,20)   | 1:40:A:SER:H     | 1:57:A:THR:HG22  | 2        | 0.15          |
| (3,9)    | 1:14:A:THR:H     | 1:111:A:GLY:HA2  | 11       | 0.15          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 13       | 0.15          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 19       | 0.15          |
| (1,1755) | 1:143:A:ILE:HA   | 1:146:A:ALA:H    | 18       | 0.15          |
| (1,1694) | 1:151:A:LEU:HD11 | 1:147:A:VAL:HA   | 2        | 0.15          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB3  | 7        | 0.15          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB1  | 18       | 0.15          |
| (1,1595) | 1:16:A:ALA:HB1   | 1:19:A:PHE:HD1   | 14       | 0.15          |
| (1,1574) | 1:128:A:ILE:HD11 | 1:91:A:ILE:HD13  | 8        | 0.15          |
| (1,1556) | 1:104:A:LEU:HD13 | 1:79:A:PHE:HB3   | 10       | 0.15          |
| (1,1432) | 1:69:A:HIS:HA    | 1:69:A:HIS:HD2   | 3        | 0.15          |
| (1,1432) | 1:69:A:HIS:HA    | 1:69:A:HIS:HD2   | 13       | 0.15          |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD12  | 1        | 0.15          |
| (1,1386) | 1:62:A:SER:HA    | 1:63:A:GLN:HE21  | 1        | 0.15          |
| (1,1302) | 1:71:A:ILE:HD13  | 1:48:A:GLY:HA2   | 8        | 0.15          |
| (1,1289) | 1:52:A:THR:HB    | 1:71:A:ILE:HG22  | 3        | 0.15          |
| (1,1211) | 1:38:A:ILE:HG21  | 1:38:A:ILE:HG12  | 5        | 0.15          |
| (1,1211) | 1:38:A:ILE:HG23  | 1:38:A:ILE:HG12  | 16       | 0.15          |
| (1,1211) | 1:38:A:ILE:HG22  | 1:38:A:ILE:HG12  | 19       | 0.15          |
| (1,1111) | 1:30:A:ILE:HA    | 1:147:A:VAL:HG11 | 1        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1109) | 1:30:A:ILE:HA   | 1:30:A:ILE:HG12 | 6        | 0.15          |
| (1,1072) | 1:23:A:VAL:HG13 | 1:23:A:VAL:H    | 4        | 0.15          |
| (1,1072) | 1:23:A:VAL:HG12 | 1:23:A:VAL:H    | 10       | 0.15          |
| (1,1072) | 1:23:A:VAL:HG12 | 1:23:A:VAL:H    | 14       | 0.15          |
| (1,1051) | 1:148:A:GLU:HB3 | 1:144:A:PHE:HB3 | 15       | 0.15          |
| (1,965)  | 1:12:A:VAL:HG21 | 1:111:A:GLY:H   | 19       | 0.15          |
| (1,950)  | 1:11:A:THR:HB   | 1:22:A:PHE:HD2  | 2        | 0.15          |
| (1,950)  | 1:11:A:THR:HB   | 1:22:A:PHE:HD2  | 9        | 0.15          |
| (1,940)  | 1:10:A:THR:HG21 | 1:107:A:SER:HB2 | 1        | 0.15          |
| (1,940)  | 1:10:A:THR:HG23 | 1:107:A:SER:HB2 | 3        | 0.15          |
| (1,905)  | 1:4:A:THR:HG21  | 1:119:A:LYS:HB2 | 5        | 0.15          |
| (1,859)  | 1:78:A:ASN:HD21 | 1:77:A:ALA:HB2  | 8        | 0.15          |
| (1,839)  | 1:154:A:ASN:H   | 1:153:A:ALA:HB2 | 4        | 0.15          |
| (1,823)  | 1:153:A:ALA:H   | 1:17:A:ARG:HH11 | 5        | 0.15          |
| (1,822)  | 1:153:A:ALA:H   | 1:151:A:LEU:H   | 13       | 0.15          |
| (1,795)  | 1:146:A:ALA:H   | 1:142:A:GLY:HA3 | 2        | 0.15          |
| (1,793)  | 1:146:A:ALA:H   | 1:143:A:ILE:HB  | 1        | 0.15          |
| (1,793)  | 1:146:A:ALA:H   | 1:143:A:ILE:HB  | 4        | 0.15          |
| (1,793)  | 1:146:A:ALA:H   | 1:143:A:ILE:HB  | 11       | 0.15          |
| (1,793)  | 1:146:A:ALA:H   | 1:143:A:ILE:HB  | 16       | 0.15          |
| (1,771)  | 1:139:A:GLU:H   | 1:136:A:GLY:H   | 7        | 0.15          |
| (1,771)  | 1:139:A:GLU:H   | 1:136:A:GLY:H   | 8        | 0.15          |
| (1,771)  | 1:139:A:GLU:H   | 1:136:A:GLY:H   | 9        | 0.15          |
| (1,771)  | 1:139:A:GLU:H   | 1:136:A:GLY:H   | 11       | 0.15          |
| (1,700)  | 1:121:A:HIS:H   | 1:85:A:LEU:HD12 | 3        | 0.15          |
| (1,640)  | 1:113:A:ILE:H   | 1:114:A:LEU:HG  | 8        | 0.15          |
| (1,540)  | 1:101:A:GLU:H   | 1:116:A:SER:HA  | 8        | 0.15          |
| (1,540)  | 1:101:A:GLU:H   | 1:116:A:SER:HA  | 10       | 0.15          |
| (1,540)  | 1:101:A:GLU:H   | 1:116:A:SER:HA  | 17       | 0.15          |
| (1,540)  | 1:101:A:GLU:H   | 1:116:A:SER:HA  | 19       | 0.15          |
| (1,505)  | 1:96:A:GLU:H    | 1:85:A:LEU:HD13 | 5        | 0.15          |
| (1,458)  | 1:82:A:ALA:H    | 1:73:A:GLU:HG3  | 1        | 0.15          |
| (1,458)  | 1:82:A:ALA:H    | 1:73:A:GLU:HG3  | 15       | 0.15          |
| (1,449)  | 1:81:A:TYR:H    | 1:19:A:PHE:HD1  | 7        | 0.15          |
| (1,404)  | 1:75:A:ASP:H    | 1:81:A:TYR:H    | 12       | 0.15          |
| (1,375)  | 1:70:A:ARG:H    | 1:54:A:LYS:HE2  | 12       | 0.15          |
| (1,373)  | 1:70:A:ARG:H    | 1:69:A:HIS:HB3  | 15       | 0.15          |
| (1,345)  | 1:64:A:PHE:H    | 1:62:A:SER:HA   | 9        | 0.15          |
| (1,310)  | 1:56:A:ILE:H    | 1:67:A:VAL:HG12 | 9        | 0.15          |
| (1,264)  | 1:88:A:GLY:H    | 1:67:A:VAL:HG21 | 11       | 0.15          |
| (1,47)   | 1:6:A:GLU:H     | 1:7:A:SER:HA    | 1        | 0.15          |
| (4,33)   | 1:87:A:GLU:H    | 1:68:A:LYS:O    | 3        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (4,33)   | 1:87:A:GLU:H     | 1:68:A:LYS:O     | 18       | 0.14          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2   | 7        | 0.14          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2   | 11       | 0.14          |
| (3,172)  | 1:101:A:GLU:HA   | 1:100:A:TYR:H    | 2        | 0.14          |
| (1,1782) | 1:157:A:ALA:HA   | 1:155:A:PRO:HD2  | 13       | 0.14          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 20       | 0.14          |
| (1,1766) | 1:9:A:THR:HB     | 1:102:A:ILE:HG22 | 6        | 0.14          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 12       | 0.14          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 14       | 0.14          |
| (1,1699) | 1:153:A:ALA:HA   | 1:154:A:ASN:HA   | 2        | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB2  | 1        | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB1  | 2        | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB1  | 3        | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB1  | 5        | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB1  | 6        | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB3  | 8        | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB2  | 9        | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB1  | 10       | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB1  | 11       | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB1  | 12       | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB3  | 13       | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB2  | 16       | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB1  | 17       | 0.14          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB3  | 20       | 0.14          |
| (1,1661) | 1:143:A:ILE:HA   | 1:37:A:ALA:HB1   | 4        | 0.14          |
| (1,1661) | 1:143:A:ILE:HA   | 1:37:A:ALA:HB2   | 17       | 0.14          |
| (1,1650) | 1:145:A:LYS:HA   | 1:148:A:GLU:HB3  | 14       | 0.14          |
| (1,1631) | 1:122:A:THR:HA   | 1:122:A:THR:HG21 | 15       | 0.14          |
| (1,1624) | 1:118:A:SER:HB2  | 1:119:A:LYS:HB2  | 15       | 0.14          |
| (1,1574) | 1:128:A:ILE:HD13 | 1:91:A:ILE:HD12  | 9        | 0.14          |
| (1,1557) | 1:85:A:LEU:HD12  | 1:91:A:ILE:HG12  | 10       | 0.14          |
| (1,1551) | 1:114:A:LEU:HA   | 1:104:A:LEU:HD23 | 1        | 0.14          |
| (1,1310) | 1:44:A:ILE:HD12  | 1:68:A:LYS:HD2   | 7        | 0.14          |
| (1,1289) | 1:52:A:THR:HB    | 1:71:A:ILE:HG23  | 16       | 0.14          |
| (1,1261) | 1:13:A:ILE:HB    | 1:18:A:LEU:HD21  | 11       | 0.14          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG23  | 9        | 0.14          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG22  | 11       | 0.14          |
| (1,1198) | 1:53:A:ILE:HB    | 1:53:A:ILE:HG23  | 13       | 0.14          |
| (1,1176) | 1:34:A:ALA:HA    | 1:30:A:ILE:HA    | 7        | 0.14          |
| (1,1149) | 1:143:A:ILE:HG12 | 1:34:A:ALA:HB2   | 3        | 0.14          |
| (1,1129) | 1:30:A:ILE:HG21  | 1:37:A:ALA:H     | 15       | 0.14          |
| (1,1109) | 1:30:A:ILE:HA    | 1:30:A:ILE:HG12  | 4        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1109) | 1:30:A:ILE:HA    | 1:30:A:ILE:HG12  | 12       | 0.14          |
| (1,1109) | 1:30:A:ILE:HA    | 1:30:A:ILE:HG12  | 14       | 0.14          |
| (1,1109) | 1:30:A:ILE:HA    | 1:30:A:ILE:HG12  | 18       | 0.14          |
| (1,1053) | 1:33:A:VAL:HG23  | 1:30:A:ILE:HA    | 20       | 0.14          |
| (1,1047) | 1:20:A:LYS:HA    | 1:23:A:VAL:HB    | 15       | 0.14          |
| (1,1029) | 1:17:A:ARG:HB3   | 1:151:A:LEU:HD12 | 7        | 0.14          |
| (1,967)  | 1:103:A:LYS:HB2  | 1:80:A:THR:HG23  | 7        | 0.14          |
| (1,943)  | 1:117:A:THR:HG23 | 1:101:A:GLU:HB3  | 11       | 0.14          |
| (1,822)  | 1:153:A:ALA:H    | 1:151:A:LEU:H    | 8        | 0.14          |
| (1,822)  | 1:153:A:ALA:H    | 1:151:A:LEU:H    | 14       | 0.14          |
| (1,822)  | 1:153:A:ALA:H    | 1:151:A:LEU:H    | 20       | 0.14          |
| (1,793)  | 1:146:A:ALA:H    | 1:143:A:ILE:HB   | 2        | 0.14          |
| (1,771)  | 1:139:A:GLU:H    | 1:136:A:GLY:H    | 13       | 0.14          |
| (1,771)  | 1:139:A:GLU:H    | 1:136:A:GLY:H    | 15       | 0.14          |
| (1,708)  | 1:122:A:THR:H    | 1:95:A:LEU:HA    | 14       | 0.14          |
| (1,648)  | 1:114:A:LEU:H    | 1:113:A:ILE:HG22 | 7        | 0.14          |
| (1,648)  | 1:114:A:LEU:H    | 1:113:A:ILE:HG23 | 14       | 0.14          |
| (1,629)  | 1:112:A:SER:H    | 1:111:A:GLY:HA2  | 5        | 0.14          |
| (1,614)  | 1:110:A:GLY:H    | 1:106:A:ALA:HB1  | 8        | 0.14          |
| (1,564)  | 1:104:A:LEU:H    | 1:104:A:LEU:HG   | 1        | 0.14          |
| (1,564)  | 1:104:A:LEU:H    | 1:104:A:LEU:HG   | 10       | 0.14          |
| (1,540)  | 1:101:A:GLU:H    | 1:116:A:SER:HA   | 5        | 0.14          |
| (1,540)  | 1:101:A:GLU:H    | 1:116:A:SER:HA   | 15       | 0.14          |
| (1,540)  | 1:101:A:GLU:H    | 1:116:A:SER:HA   | 16       | 0.14          |
| (1,520)  | 1:97:A:LYS:H     | 1:121:A:HIS:HB3  | 4        | 0.14          |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 14       | 0.14          |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 19       | 0.14          |
| (1,494)  | 1:91:A:ILE:H     | 1:91:A:ILE:HG13  | 20       | 0.14          |
| (1,458)  | 1:82:A:ALA:H     | 1:73:A:GLU:HG3   | 9        | 0.14          |
| (1,404)  | 1:75:A:ASP:H     | 1:81:A:TYR:H     | 6        | 0.14          |
| (1,375)  | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 8        | 0.14          |
| (1,334)  | 1:59:A:GLY:H     | 1:58:A:PHE:HB2   | 13       | 0.14          |
| (1,310)  | 1:56:A:ILE:H     | 1:67:A:VAL:HG13  | 13       | 0.14          |
| (1,307)  | 1:55:A:LYS:H     | 1:55:A:LYS:HG2   | 14       | 0.14          |
| (1,195)  | 1:36:A:GLN:H     | 1:36:A:GLN:HB2   | 20       | 0.14          |
| (4,64)   | 1:139:A:GLU:N    | 1:135:A:ALA:O    | 19       | 0.13          |
| (4,34)   | 1:87:A:GLU:N     | 1:68:A:LYS:O     | 19       | 0.13          |
| (4,33)   | 1:87:A:GLU:H     | 1:68:A:LYS:O     | 16       | 0.13          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2   | 17       | 0.13          |
| (1,1782) | 1:157:A:ALA:HA   | 1:155:A:PRO:HD2  | 19       | 0.13          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 2        | 0.13          |
| (1,1781) | 1:157:A:ALA:HA   | 1:158:A:TYR:HA   | 7        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1771) | 1:150:A:TYR:HA   | 1:154:A:ASN:HD22 | 7        | 0.13          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 1        | 0.13          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H    | 17       | 0.13          |
| (1,1755) | 1:143:A:ILE:HA   | 1:146:A:ALA:H    | 3        | 0.13          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB3  | 4        | 0.13          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB2  | 14       | 0.13          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB3  | 19       | 0.13          |
| (1,1626) | 1:118:A:SER:HB2  | 1:117:A:THR:HG22 | 2        | 0.13          |
| (1,1574) | 1:128:A:ILE:HD12 | 1:91:A:ILE:HD12  | 1        | 0.13          |
| (1,1557) | 1:85:A:LEU:HD12  | 1:91:A:ILE:HG12  | 14       | 0.13          |
| (1,1537) | 1:128:A:ILE:HD11 | 1:120:A:TYR:HB3  | 11       | 0.13          |
| (1,1514) | 1:18:A:LEU:HD22  | 1:13:A:ILE:HA    | 15       | 0.13          |
| (1,1429) | 1:104:A:LEU:HD11 | 1:106:A:ALA:H    | 8        | 0.13          |
| (1,1385) | 1:62:A:SER:HA    | 1:60:A:GLU:H     | 13       | 0.13          |
| (1,1383) | 1:130:A:GLU:HG2  | 1:133:A:ILE:HG12 | 3        | 0.13          |
| (1,1351) | 1:56:A:ILE:HG22  | 1:38:A:ILE:HG23  | 12       | 0.13          |
| (1,1344) | 1:128:A:ILE:HG13 | 1:3:A:PHE:HB3    | 19       | 0.13          |
| (1,1340) | 1:128:A:ILE:HD12 | 1:98:A:ILE:HG22  | 10       | 0.13          |
| (1,1289) | 1:52:A:THR:HB    | 1:71:A:ILE:HG21  | 15       | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 1        | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 2        | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 3        | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 4        | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 5        | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 6        | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 7        | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 8        | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 9        | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 10       | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 11       | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 12       | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 13       | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 14       | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 15       | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 16       | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 17       | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 18       | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 19       | 0.13          |
| (1,1266) | 1:46:A:GLY:HA2   | 1:46:A:GLY:HA3   | 20       | 0.13          |
| (1,1239) | 1:43:A:ILE:HD12  | 1:43:A:ILE:HB    | 15       | 0.13          |
| (1,1200) | 1:38:A:ILE:HD12  | 1:38:A:ILE:HB    | 12       | 0.13          |
| (1,1196) | 1:139:A:GLU:HA   | 1:142:A:GLY:H    | 5        | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1171) | 1:33:A:VAL:HG23 | 1:29:A:LEU:HB2   | 3        | 0.13          |
| (1,1155) | 1:32:A:LYS:HA   | 1:32:A:LYS:HD3   | 2        | 0.13          |
| (1,1140) | 1:31:A:PRO:HA   | 1:37:A:ALA:H     | 3        | 0.13          |
| (1,1131) | 1:91:A:ILE:HG21 | 1:96:A:GLU:H     | 18       | 0.13          |
| (1,1109) | 1:30:A:ILE:HA   | 1:30:A:ILE:HG12  | 1        | 0.13          |
| (1,1109) | 1:30:A:ILE:HA   | 1:30:A:ILE:HG12  | 13       | 0.13          |
| (1,1109) | 1:30:A:ILE:HA   | 1:30:A:ILE:HG12  | 17       | 0.13          |
| (1,1029) | 1:17:A:ARG:HB3  | 1:151:A:LEU:HD13 | 11       | 0.13          |
| (1,1029) | 1:17:A:ARG:HB3  | 1:151:A:LEU:HD11 | 17       | 0.13          |
| (1,976)  | 1:13:A:ILE:HG21 | 1:17:A:ARG:HB2   | 5        | 0.13          |
| (1,976)  | 1:13:A:ILE:HG21 | 1:17:A:ARG:HB2   | 15       | 0.13          |
| (1,940)  | 1:10:A:THR:HG23 | 1:107:A:SER:HB2  | 5        | 0.13          |
| (1,939)  | 1:80:A:THR:HG23 | 1:74:A:ILE:HA    | 10       | 0.13          |
| (1,840)  | 1:154:A:ASN:H   | 1:154:A:ASN:HB3  | 6        | 0.13          |
| (1,839)  | 1:154:A:ASN:H   | 1:153:A:ALA:HB3  | 12       | 0.13          |
| (1,823)  | 1:153:A:ALA:H   | 1:17:A:ARG:HH11  | 15       | 0.13          |
| (1,822)  | 1:153:A:ALA:H   | 1:151:A:LEU:H    | 12       | 0.13          |
| (1,822)  | 1:153:A:ALA:H   | 1:151:A:LEU:H    | 19       | 0.13          |
| (1,793)  | 1:146:A:ALA:H   | 1:143:A:ILE:HB   | 17       | 0.13          |
| (1,793)  | 1:146:A:ALA:H   | 1:143:A:ILE:HB   | 19       | 0.13          |
| (1,668)  | 1:116:A:SER:H   | 1:8:A:GLU:HB3    | 8        | 0.13          |
| (1,657)  | 1:115:A:LYS:H   | 1:115:A:LYS:HB3  | 10       | 0.13          |
| (1,648)  | 1:114:A:LEU:H   | 1:113:A:ILE:HG23 | 12       | 0.13          |
| (1,648)  | 1:114:A:LEU:H   | 1:113:A:ILE:HG21 | 20       | 0.13          |
| (1,640)  | 1:113:A:ILE:H   | 1:114:A:LEU:HG   | 3        | 0.13          |
| (1,640)  | 1:113:A:ILE:H   | 1:114:A:LEU:HG   | 11       | 0.13          |
| (1,640)  | 1:113:A:ILE:H   | 1:114:A:LEU:HG   | 16       | 0.13          |
| (1,629)  | 1:112:A:SER:H   | 1:111:A:GLY:HA2  | 13       | 0.13          |
| (1,614)  | 1:110:A:GLY:H   | 1:106:A:ALA:HB2  | 15       | 0.13          |
| (1,540)  | 1:101:A:GLU:H   | 1:116:A:SER:HA   | 1        | 0.13          |
| (1,540)  | 1:101:A:GLU:H   | 1:116:A:SER:HA   | 11       | 0.13          |
| (1,540)  | 1:101:A:GLU:H   | 1:116:A:SER:HA   | 13       | 0.13          |
| (1,520)  | 1:97:A:LYS:H    | 1:121:A:HIS:HB3  | 8        | 0.13          |
| (1,518)  | 1:97:A:LYS:H    | 1:85:A:LEU:HD12  | 11       | 0.13          |
| (1,518)  | 1:97:A:LYS:H    | 1:85:A:LEU:HD13  | 14       | 0.13          |
| (1,479)  | 1:87:A:GLU:H    | 1:68:A:LYS:HB3   | 5        | 0.13          |
| (1,449)  | 1:81:A:TYR:H    | 1:19:A:PHE:HD2   | 2        | 0.13          |
| (1,449)  | 1:81:A:TYR:H    | 1:19:A:PHE:HD1   | 16       | 0.13          |
| (1,404)  | 1:75:A:ASP:H    | 1:81:A:TYR:H     | 5        | 0.13          |
| (1,404)  | 1:75:A:ASP:H    | 1:81:A:TYR:H     | 7        | 0.13          |
| (1,404)  | 1:75:A:ASP:H    | 1:81:A:TYR:H     | 16       | 0.13          |
| (1,404)  | 1:75:A:ASP:H    | 1:81:A:TYR:H     | 18       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,404)  | 1:75:A:ASP:H     | 1:81:A:TYR:H     | 19       | 0.13          |
| (1,347)  | 1:66:A:TYR:H     | 1:65:A:ASN:HB2   | 8        | 0.13          |
| (1,307)  | 1:55:A:LYS:H     | 1:55:A:LYS:HG2   | 2        | 0.13          |
| (1,307)  | 1:55:A:LYS:H     | 1:55:A:LYS:HG2   | 3        | 0.13          |
| (1,307)  | 1:55:A:LYS:H     | 1:55:A:LYS:HG2   | 9        | 0.13          |
| (1,128)  | 1:18:A:LEU:H     | 1:13:A:ILE:HG23  | 13       | 0.13          |
| (1,66)   | 1:9:A:THR:H      | 1:116:A:SER:HA   | 1        | 0.13          |
| (1,47)   | 1:6:A:GLU:H      | 1:7:A:SER:HA     | 7        | 0.13          |
| (4,52)   | 1:113:A:ILE:N    | 1:105:A:VAL:O    | 8        | 0.12          |
| (4,34)   | 1:87:A:GLU:N     | 1:68:A:LYS:O     | 1        | 0.12          |
| (4,34)   | 1:87:A:GLU:N     | 1:68:A:LYS:O     | 6        | 0.12          |
| (4,33)   | 1:87:A:GLU:H     | 1:68:A:LYS:O     | 5        | 0.12          |
| (4,33)   | 1:87:A:GLU:H     | 1:68:A:LYS:O     | 11       | 0.12          |
| (4,1)    | 1:3:A:PHE:H      | 1:120:A:TYR:O    | 17       | 0.12          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2   | 16       | 0.12          |
| (3,172)  | 1:101:A:GLU:HA   | 1:100:A:TYR:H    | 5        | 0.12          |
| (3,153)  | 1:113:A:ILE:HD11 | 1:108:A:PRO:HG2  | 18       | 0.12          |
| (3,149)  | 1:4:A:THR:HG21   | 1:6:A:GLU:HB2    | 13       | 0.12          |
| (3,135)  | 1:115:A:LYS:HD3  | 1:8:A:GLU:HA     | 1        | 0.12          |
| (1,1766) | 1:9:A:THR:HB     | 1:102:A:ILE:HG23 | 15       | 0.12          |
| (1,1735) | 1:84:A:THR:HA    | 1:99:A:ALA:HA    | 18       | 0.12          |
| (1,1681) | 1:149:A:ALA:HA   | 1:149:A:ALA:HB2  | 15       | 0.12          |
| (1,1650) | 1:145:A:LYS:HA   | 1:148:A:GLU:HB3  | 5        | 0.12          |
| (1,1551) | 1:114:A:LEU:HA   | 1:104:A:LEU:HD21 | 9        | 0.12          |
| (1,1474) | 1:79:A:PHE:HB3   | 1:104:A:LEU:HB3  | 12       | 0.12          |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD13  | 15       | 0.12          |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD11  | 19       | 0.12          |
| (1,1385) | 1:62:A:SER:HA    | 1:60:A:GLU:H     | 3        | 0.12          |
| (1,1385) | 1:62:A:SER:HA    | 1:60:A:GLU:H     | 15       | 0.12          |
| (1,1340) | 1:128:A:ILE:HD13 | 1:98:A:ILE:HG21  | 12       | 0.12          |
| (1,1302) | 1:71:A:ILE:HD12  | 1:48:A:GLY:HA2   | 20       | 0.12          |
| (1,1238) | 1:43:A:ILE:HD13  | 1:48:A:GLY:HA2   | 8        | 0.12          |
| (1,1233) | 1:133:A:ILE:HG13 | 1:128:A:ILE:HB   | 7        | 0.12          |
| (1,1232) | 1:133:A:ILE:HG13 | 1:132:A:GLN:HB2  | 6        | 0.12          |
| (1,1200) | 1:38:A:ILE:HD12  | 1:38:A:ILE:HB    | 7        | 0.12          |
| (1,1200) | 1:38:A:ILE:HD11  | 1:38:A:ILE:HB    | 19       | 0.12          |
| (1,1134) | 1:30:A:ILE:HG21  | 1:37:A:ALA:HB3   | 13       | 0.12          |
| (1,1133) | 1:91:A:ILE:HG23  | 1:95:A:LEU:HB3   | 6        | 0.12          |
| (1,1121) | 1:74:A:ILE:HD12  | 1:19:A:PHE:HD2   | 8        | 0.12          |
| (1,1120) | 1:74:A:ILE:HD12  | 1:71:A:ILE:HA    | 10       | 0.12          |
| (1,1120) | 1:74:A:ILE:HD13  | 1:71:A:ILE:HA    | 19       | 0.12          |
| (1,1111) | 1:30:A:ILE:HA    | 1:147:A:VAL:HG11 | 6        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1109) | 1:30:A:ILE:HA   | 1:30:A:ILE:HG12  | 10       | 0.12          |
| (1,1109) | 1:30:A:ILE:HA   | 1:30:A:ILE:HG12  | 11       | 0.12          |
| (1,1109) | 1:30:A:ILE:HA   | 1:30:A:ILE:HG12  | 16       | 0.12          |
| (1,1072) | 1:23:A:VAL:HG13 | 1:23:A:VAL:H     | 17       | 0.12          |
| (1,1043) | 1:18:A:LEU:HD23 | 1:22:A:PHE:HD2   | 12       | 0.12          |
| (1,1029) | 1:17:A:ARG:HB3  | 1:151:A:LEU:HD12 | 1        | 0.12          |
| (1,967)  | 1:103:A:LYS:HB2 | 1:80:A:THR:HG23  | 9        | 0.12          |
| (1,967)  | 1:103:A:LYS:HB2 | 1:80:A:THR:HG21  | 19       | 0.12          |
| (1,950)  | 1:11:A:THR:HB   | 1:22:A:PHE:HD2   | 18       | 0.12          |
| (1,940)  | 1:10:A:THR:HG22 | 1:107:A:SER:HB2  | 10       | 0.12          |
| (1,939)  | 1:80:A:THR:HG23 | 1:74:A:ILE:HA    | 1        | 0.12          |
| (1,839)  | 1:154:A:ASN:H   | 1:153:A:ALA:HB1  | 19       | 0.12          |
| (1,826)  | 1:153:A:ALA:H   | 1:151:A:LEU:HB3  | 5        | 0.12          |
| (1,822)  | 1:153:A:ALA:H   | 1:151:A:LEU:H    | 9        | 0.12          |
| (1,793)  | 1:146:A:ALA:H   | 1:143:A:ILE:HB   | 5        | 0.12          |
| (1,793)  | 1:146:A:ALA:H   | 1:143:A:ILE:HB   | 14       | 0.12          |
| (1,771)  | 1:139:A:GLU:H   | 1:136:A:GLY:H    | 1        | 0.12          |
| (1,771)  | 1:139:A:GLU:H   | 1:136:A:GLY:H    | 2        | 0.12          |
| (1,771)  | 1:139:A:GLU:H   | 1:136:A:GLY:H    | 6        | 0.12          |
| (1,771)  | 1:139:A:GLU:H   | 1:136:A:GLY:H    | 14       | 0.12          |
| (1,657)  | 1:115:A:LYS:H   | 1:115:A:LYS:HB3  | 19       | 0.12          |
| (1,648)  | 1:114:A:LEU:H   | 1:113:A:ILE:HG21 | 6        | 0.12          |
| (1,640)  | 1:113:A:ILE:H   | 1:114:A:LEU:HG   | 4        | 0.12          |
| (1,640)  | 1:113:A:ILE:H   | 1:114:A:LEU:HG   | 13       | 0.12          |
| (1,614)  | 1:110:A:GLY:H   | 1:106:A:ALA:HB2  | 10       | 0.12          |
| (1,564)  | 1:104:A:LEU:H   | 1:104:A:LEU:HG   | 19       | 0.12          |
| (1,540)  | 1:101:A:GLU:H   | 1:116:A:SER:HA   | 2        | 0.12          |
| (1,540)  | 1:101:A:GLU:H   | 1:116:A:SER:HA   | 7        | 0.12          |
| (1,477)  | 1:87:A:GLU:H    | 1:67:A:VAL:HG22  | 10       | 0.12          |
| (1,449)  | 1:81:A:TYR:H    | 1:19:A:PHE:HD1   | 5        | 0.12          |
| (1,404)  | 1:75:A:ASP:H    | 1:81:A:TYR:H     | 10       | 0.12          |
| (1,404)  | 1:75:A:ASP:H    | 1:81:A:TYR:H     | 11       | 0.12          |
| (1,404)  | 1:75:A:ASP:H    | 1:81:A:TYR:H     | 14       | 0.12          |
| (1,98)   | 1:157:A:ALA:H   | 1:154:A:ASN:HA   | 5        | 0.12          |
| (1,98)   | 1:157:A:ALA:H   | 1:154:A:ASN:HA   | 7        | 0.12          |
| (1,98)   | 1:157:A:ALA:H   | 1:154:A:ASN:HA   | 20       | 0.12          |
| (1,66)   | 1:9:A:THR:H     | 1:116:A:SER:HA   | 11       | 0.12          |
| (1,66)   | 1:9:A:THR:H     | 1:116:A:SER:HA   | 14       | 0.12          |
| (1,66)   | 1:9:A:THR:H     | 1:116:A:SER:HA   | 15       | 0.12          |
| (1,47)   | 1:6:A:GLU:H     | 1:7:A:SER:HA     | 12       | 0.12          |
| (4,80)   | 1:151:A:LEU:N   | 1:147:A:VAL:O    | 2        | 0.11          |
| (4,65)   | 1:140:A:ALA:H   | 1:136:A:GLY:O    | 12       | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (4,64)   | 1:139:A:GLU:N    | 1:135:A:ALA:O   | 18       | 0.11          |
| (4,62)   | 1:138:A:GLU:N    | 1:134:A:LYS:O   | 13       | 0.11          |
| (4,54)   | 1:134:A:LYS:N    | 1:130:A:GLU:O   | 7        | 0.11          |
| (4,34)   | 1:87:A:GLU:N     | 1:68:A:LYS:O    | 7        | 0.11          |
| (4,34)   | 1:87:A:GLU:N     | 1:68:A:LYS:O    | 18       | 0.11          |
| (4,34)   | 1:87:A:GLU:N     | 1:68:A:LYS:O    | 20       | 0.11          |
| (4,33)   | 1:87:A:GLU:H     | 1:68:A:LYS:O    | 12       | 0.11          |
| (4,32)   | 1:68:A:LYS:N     | 1:87:A:GLU:O    | 6        | 0.11          |
| (4,19)   | 1:56:A:ILE:H     | 1:67:A:VAL:O    | 5        | 0.11          |
| (3,174)  | 1:55:A:LYS:HA    | 1:42:A:GLU:HB2  | 18       | 0.11          |
| (3,172)  | 1:101:A:GLU:HA   | 1:100:A:TYR:H   | 8        | 0.11          |
| (3,127)  | 1:5:A:TYR:HB2    | 1:6:A:GLU:HG2   | 16       | 0.11          |
| (1,1782) | 1:157:A:ALA:HA   | 1:155:A:PRO:HD2 | 2        | 0.11          |
| (1,1782) | 1:157:A:ALA:HA   | 1:155:A:PRO:HD2 | 16       | 0.11          |
| (1,1757) | 1:146:A:ALA:HA   | 1:150:A:TYR:H   | 3        | 0.11          |
| (1,1755) | 1:143:A:ILE:HA   | 1:146:A:ALA:H   | 1        | 0.11          |
| (1,1750) | 1:139:A:GLU:HA   | 1:141:A:SER:H   | 3        | 0.11          |
| (1,1736) | 1:101:A:GLU:HA   | 1:81:A:TYR:H    | 7        | 0.11          |
| (1,1735) | 1:84:A:THR:HA    | 1:99:A:ALA:HA   | 12       | 0.11          |
| (1,1694) | 1:151:A:LEU:HD13 | 1:147:A:VAL:HA  | 8        | 0.11          |
| (1,1661) | 1:143:A:ILE:HA   | 1:37:A:ALA:HB3  | 14       | 0.11          |
| (1,1654) | 1:133:A:ILE:HG22 | 1:5:A:TYR:HB2   | 17       | 0.11          |
| (1,1579) | 1:104:A:LEU:HA   | 1:104:A:LEU:HG  | 12       | 0.11          |
| (1,1574) | 1:128:A:ILE:HD11 | 1:91:A:ILE:HD11 | 13       | 0.11          |
| (1,1563) | 1:108:A:PRO:HB3  | 1:109:A:ASP:HB2 | 1        | 0.11          |
| (1,1537) | 1:128:A:ILE:HD13 | 1:120:A:TYR:HB3 | 7        | 0.11          |
| (1,1456) | 1:127:A:GLU:HG3  | 1:127:A:GLU:H   | 5        | 0.11          |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD12 | 10       | 0.11          |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD11 | 13       | 0.11          |
| (1,1386) | 1:62:A:SER:HA    | 1:63:A:GLN:HE21 | 3        | 0.11          |
| (1,1385) | 1:62:A:SER:HA    | 1:60:A:GLU:H    | 1        | 0.11          |
| (1,1351) | 1:56:A:ILE:HG21  | 1:38:A:ILE:HG22 | 18       | 0.11          |
| (1,1336) | 1:128:A:ILE:HD11 | 1:120:A:TYR:HB2 | 11       | 0.11          |
| (1,1300) | 1:71:A:ILE:HD12  | 1:70:A:ARG:HE   | 3        | 0.11          |
| (1,1300) | 1:71:A:ILE:HD11  | 1:70:A:ARG:HE   | 12       | 0.11          |
| (1,1271) | 1:48:A:GLY:HA2   | 1:71:A:ILE:HG12 | 14       | 0.11          |
| (1,1239) | 1:43:A:ILE:HD11  | 1:43:A:ILE:HB   | 5        | 0.11          |
| (1,1199) | 1:38:A:ILE:HD12  | 1:56:A:ILE:HG23 | 13       | 0.11          |
| (1,1166) | 1:33:A:VAL:HG12  | 1:29:A:LEU:H    | 12       | 0.11          |
| (1,1072) | 1:23:A:VAL:HG13  | 1:23:A:VAL:H    | 8        | 0.11          |
| (1,1072) | 1:23:A:VAL:HG13  | 1:23:A:VAL:H    | 15       | 0.11          |
| (1,1054) | 1:22:A:PHE:HA    | 1:29:A:LEU:HD13 | 9        | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,994) | 1:82:A:ALA:HB1   | 1:71:A:ILE:HA    | 19       | 0.11          |
| (1,967) | 1:103:A:LYS:HB2  | 1:80:A:THR:HG23  | 2        | 0.11          |
| (1,967) | 1:103:A:LYS:HB2  | 1:80:A:THR:HG21  | 3        | 0.11          |
| (1,967) | 1:103:A:LYS:HB2  | 1:80:A:THR:HG23  | 5        | 0.11          |
| (1,967) | 1:103:A:LYS:HB2  | 1:80:A:THR:HG22  | 14       | 0.11          |
| (1,950) | 1:11:A:THR:HB    | 1:22:A:PHE:HD2   | 8        | 0.11          |
| (1,943) | 1:117:A:THR:HG23 | 1:101:A:GLU:HB3  | 12       | 0.11          |
| (1,940) | 1:10:A:THR:HG23  | 1:107:A:SER:HB2  | 4        | 0.11          |
| (1,859) | 1:78:A:ASN:HD21  | 1:77:A:ALA:HB1   | 18       | 0.11          |
| (1,837) | 1:154:A:ASN:H    | 1:149:A:ALA:HA   | 19       | 0.11          |
| (1,833) | 1:154:A:ASN:H    | 1:17:A:ARG:HH11  | 9        | 0.11          |
| (1,822) | 1:153:A:ALA:H    | 1:151:A:LEU:H    | 2        | 0.11          |
| (1,822) | 1:153:A:ALA:H    | 1:151:A:LEU:H    | 16       | 0.11          |
| (1,813) | 1:148:A:GLU:H    | 1:147:A:VAL:HG22 | 2        | 0.11          |
| (1,793) | 1:146:A:ALA:H    | 1:143:A:ILE:HB   | 6        | 0.11          |
| (1,793) | 1:146:A:ALA:H    | 1:143:A:ILE:HB   | 7        | 0.11          |
| (1,793) | 1:146:A:ALA:H    | 1:143:A:ILE:HB   | 12       | 0.11          |
| (1,793) | 1:146:A:ALA:H    | 1:143:A:ILE:HB   | 15       | 0.11          |
| (1,793) | 1:146:A:ALA:H    | 1:143:A:ILE:HB   | 20       | 0.11          |
| (1,771) | 1:139:A:GLU:H    | 1:136:A:GLY:H    | 16       | 0.11          |
| (1,730) | 1:129:A:LYS:H    | 1:127:A:GLU:HA   | 2        | 0.11          |
| (1,648) | 1:114:A:LEU:H    | 1:113:A:ILE:HG23 | 4        | 0.11          |
| (1,648) | 1:114:A:LEU:H    | 1:113:A:ILE:HG23 | 5        | 0.11          |
| (1,648) | 1:114:A:LEU:H    | 1:113:A:ILE:HG21 | 15       | 0.11          |
| (1,648) | 1:114:A:LEU:H    | 1:113:A:ILE:HG23 | 19       | 0.11          |
| (1,642) | 1:113:A:ILE:H    | 1:105:A:VAL:HG11 | 1        | 0.11          |
| (1,640) | 1:113:A:ILE:H    | 1:114:A:LEU:HG   | 6        | 0.11          |
| (1,640) | 1:113:A:ILE:H    | 1:114:A:LEU:HG   | 10       | 0.11          |
| (1,640) | 1:113:A:ILE:H    | 1:114:A:LEU:HG   | 18       | 0.11          |
| (1,619) | 1:110:A:GLY:H    | 1:109:A:ASP:HA   | 6        | 0.11          |
| (1,614) | 1:110:A:GLY:H    | 1:106:A:ALA:HB2  | 11       | 0.11          |
| (1,564) | 1:104:A:LEU:H    | 1:104:A:LEU:HG   | 12       | 0.11          |
| (1,487) | 1:29:A:LEU:H     | 1:28:A:ASN:HA    | 6        | 0.11          |
| (1,449) | 1:81:A:TYR:H     | 1:19:A:PHE:HD1   | 9        | 0.11          |
| (1,404) | 1:75:A:ASP:H     | 1:81:A:TYR:H     | 2        | 0.11          |
| (1,404) | 1:75:A:ASP:H     | 1:81:A:TYR:H     | 4        | 0.11          |
| (1,375) | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 16       | 0.11          |
| (1,373) | 1:70:A:ARG:H     | 1:69:A:HIS:HB3   | 8        | 0.11          |
| (1,344) | 1:64:A:PHE:H     | 1:57:A:THR:HG22  | 7        | 0.11          |
| (1,343) | 1:63:A:GLN:HE22  | 1:63:A:GLN:HA    | 3        | 0.11          |
| (1,334) | 1:59:A:GLY:H     | 1:58:A:PHE:HB2   | 1        | 0.11          |
| (1,307) | 1:55:A:LYS:H     | 1:55:A:LYS:HG2   | 6        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,307)  | 1:55:A:LYS:H     | 1:55:A:LYS:HG2   | 17       | 0.11          |
| (1,292)  | 1:52:A:THR:H     | 1:46:A:GLY:HA2   | 6        | 0.11          |
| (1,98)   | 1:157:A:ALA:H    | 1:154:A:ASN:HA   | 15       | 0.11          |
| (1,95)   | 1:13:A:ILE:H     | 1:12:A:VAL:HG12  | 13       | 0.11          |
| (1,66)   | 1:9:A:THR:H      | 1:116:A:SER:HA   | 7        | 0.11          |
| (1,66)   | 1:9:A:THR:H      | 1:116:A:SER:HA   | 9        | 0.11          |
| (1,66)   | 1:9:A:THR:H      | 1:116:A:SER:HA   | 13       | 0.11          |
| (1,47)   | 1:6:A:GLU:H      | 1:7:A:SER:HA     | 6        | 0.11          |
| (1,47)   | 1:6:A:GLU:H      | 1:7:A:SER:HA     | 11       | 0.11          |
| (1,47)   | 1:6:A:GLU:H      | 1:7:A:SER:HA     | 14       | 0.11          |
| (1,40)   | 1:5:A:TYR:H      | 1:119:A:LYS:HG2  | 18       | 0.11          |
| (4,64)   | 1:139:A:GLU:N    | 1:135:A:ALA:O    | 4        | 0.1           |
| (4,64)   | 1:139:A:GLU:N    | 1:135:A:ALA:O    | 5        | 0.1           |
| (4,64)   | 1:139:A:GLU:N    | 1:135:A:ALA:O    | 11       | 0.1           |
| (4,52)   | 1:113:A:ILE:N    | 1:105:A:VAL:O    | 7        | 0.1           |
| (4,52)   | 1:113:A:ILE:N    | 1:105:A:VAL:O    | 11       | 0.1           |
| (4,34)   | 1:87:A:GLU:N     | 1:68:A:LYS:O     | 3        | 0.1           |
| (4,34)   | 1:87:A:GLU:N     | 1:68:A:LYS:O     | 16       | 0.1           |
| (4,33)   | 1:87:A:GLU:H     | 1:68:A:LYS:O     | 17       | 0.1           |
| (4,32)   | 1:68:A:LYS:N     | 1:87:A:GLU:O     | 20       | 0.1           |
| (4,26)   | 1:69:A:HIS:N     | 1:54:A:LYS:O     | 9        | 0.1           |
| (3,157)  | 1:114:A:LEU:HD21 | 1:22:A:PHE:HD1   | 4        | 0.1           |
| (1,1782) | 1:157:A:ALA:HA   | 1:155:A:PRO:HD2  | 12       | 0.1           |
| (1,1771) | 1:150:A:TYR:HA   | 1:154:A:ASN:HD22 | 17       | 0.1           |
| (1,1755) | 1:143:A:ILE:HA   | 1:146:A:ALA:H    | 17       | 0.1           |
| (1,1733) | 1:103:A:LYS:HA   | 1:80:A:THR:HA    | 1        | 0.1           |
| (1,1650) | 1:145:A:LYS:HA   | 1:148:A:GLU:HB3  | 2        | 0.1           |
| (1,1432) | 1:69:A:HIS:HA    | 1:69:A:HIS:HD2   | 5        | 0.1           |
| (1,1411) | 1:98:A:ILE:HA    | 1:85:A:LEU:HD13  | 2        | 0.1           |
| (1,1281) | 1:155:A:PRO:HD3  | 1:151:A:LEU:HD22 | 7        | 0.1           |
| (1,1281) | 1:155:A:PRO:HD3  | 1:151:A:LEU:HD23 | 11       | 0.1           |
| (1,1261) | 1:13:A:ILE:HB    | 1:18:A:LEU:HD22  | 10       | 0.1           |
| (1,1231) | 1:98:A:ILE:HG22  | 1:85:A:LEU:HD13  | 18       | 0.1           |
| (1,1219) | 1:41:A:SER:HA    | 1:56:A:ILE:HA    | 10       | 0.1           |
| (1,1208) | 1:38:A:ILE:HG21  | 1:30:A:ILE:HB    | 10       | 0.1           |
| (1,1200) | 1:38:A:ILE:HD12  | 1:38:A:ILE:HB    | 5        | 0.1           |
| (1,1200) | 1:38:A:ILE:HD13  | 1:38:A:ILE:HB    | 16       | 0.1           |
| (1,1168) | 1:33:A:VAL:HG12  | 1:150:A:TYR:HB3  | 7        | 0.1           |
| (1,1072) | 1:23:A:VAL:HG11  | 1:23:A:VAL:H     | 11       | 0.1           |
| (1,950)  | 1:11:A:THR:HB    | 1:22:A:PHE:HD2   | 10       | 0.1           |
| (1,876)  | 1:132:A:GLN:HE22 | 1:132:A:GLN:HE21 | 5        | 0.1           |
| (1,876)  | 1:132:A:GLN:HE22 | 1:132:A:GLN:HE21 | 14       | 0.1           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,876) | 1:132:A:GLN:HE22 | 1:132:A:GLN:HE21 | 16       | 0.1           |
| (1,793) | 1:146:A:ALA:H    | 1:143:A:ILE:HB   | 8        | 0.1           |
| (1,793) | 1:146:A:ALA:H    | 1:143:A:ILE:HB   | 9        | 0.1           |
| (1,771) | 1:139:A:GLU:H    | 1:136:A:GLY:H    | 5        | 0.1           |
| (1,720) | 1:128:A:ILE:H    | 1:128:A:ILE:HG13 | 7        | 0.1           |
| (1,708) | 1:122:A:THR:H    | 1:95:A:LEU:HA    | 11       | 0.1           |
| (1,640) | 1:113:A:ILE:H    | 1:114:A:LEU:HG   | 9        | 0.1           |
| (1,640) | 1:113:A:ILE:H    | 1:114:A:LEU:HG   | 19       | 0.1           |
| (1,564) | 1:104:A:LEU:H    | 1:104:A:LEU:HG   | 11       | 0.1           |
| (1,477) | 1:87:A:GLU:H     | 1:67:A:VAL:HG23  | 1        | 0.1           |
| (1,449) | 1:81:A:TYR:H     | 1:19:A:PHE:HD2   | 14       | 0.1           |
| (1,449) | 1:81:A:TYR:H     | 1:19:A:PHE:HD1   | 20       | 0.1           |
| (1,375) | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 2        | 0.1           |
| (1,375) | 1:70:A:ARG:H     | 1:54:A:LYS:HE2   | 11       | 0.1           |
| (1,344) | 1:64:A:PHE:H     | 1:57:A:THR:HG21  | 10       | 0.1           |
| (1,307) | 1:55:A:LYS:H     | 1:55:A:LYS:HG2   | 16       | 0.1           |
| (1,307) | 1:55:A:LYS:H     | 1:55:A:LYS:HG2   | 20       | 0.1           |
| (1,95)  | 1:13:A:ILE:H     | 1:12:A:VAL:HG13  | 11       | 0.1           |
| (1,47)  | 1:6:A:GLU:H      | 1:7:A:SER:HA     | 9        | 0.1           |

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

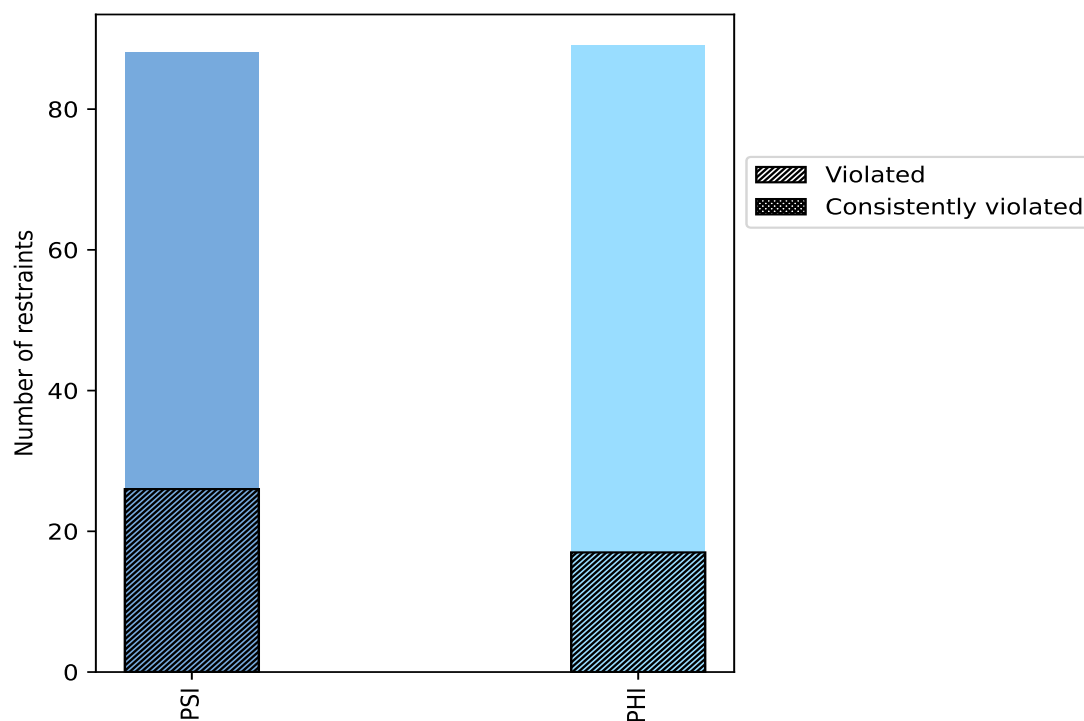
### 10.1 Summary of dihedral-angle violations [i](#)

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        | 88    | 49.7           | 26                    | 29.5           | 14.7           | 0                                  | 0.0            | 0.0            |
| PHI        | 89    | 50.3           | 17                    | 19.1           | 9.6            | 0                                  | 0.0            | 0.0            |
| Total      | 177   | 100.0          | 43                    | 24.3           | 24.3           | 0                                  | 0.0            | 0.0            |

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

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



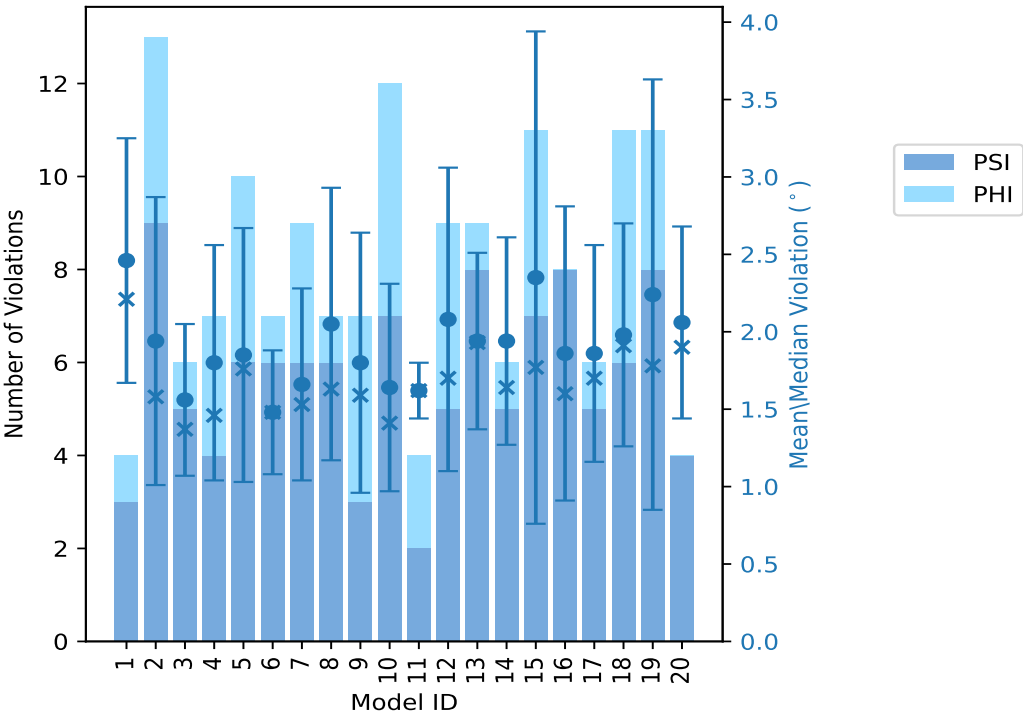
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 3                    | 1   | 4     | 2.46     | 3.71    | 0.79   | 2.21       |
| 2        | 9                    | 4   | 13    | 1.94     | 3.95    | 0.93   | 1.58       |
| 3        | 5                    | 1   | 6     | 1.56     | 2.47    | 0.49   | 1.37       |
| 4        | 4                    | 3   | 7     | 1.8      | 3.26    | 0.76   | 1.46       |
| 5        | 6                    | 4   | 10    | 1.85     | 3.83    | 0.82   | 1.76       |
| 6        | 6                    | 1   | 7     | 1.48     | 2.12    | 0.4    | 1.48       |
| 7        | 6                    | 3   | 9     | 1.66     | 3.02    | 0.62   | 1.53       |
| 8        | 6                    | 1   | 7     | 2.05     | 3.66    | 0.88   | 1.63       |
| 9        | 3                    | 4   | 7     | 1.8      | 3.77    | 0.84   | 1.59       |
| 10       | 7                    | 5   | 12    | 1.64     | 3.32    | 0.67   | 1.41       |
| 11       | 2                    | 2   | 4     | 1.62     | 1.86    | 0.18   | 1.62       |
| 12       | 5                    | 4   | 9     | 2.08     | 4.18    | 0.98   | 1.7        |
| 13       | 8                    | 1   | 9     | 1.94     | 3.01    | 0.57   | 1.93       |
| 14       | 5                    | 1   | 6     | 1.94     | 2.93    | 0.67   | 1.64       |
| 15       | 7                    | 4   | 11    | 2.35     | 7.09    | 1.59   | 1.77       |
| 16       | 8                    | 0   | 8     | 1.86     | 4.13    | 0.95   | 1.6        |
| 17       | 5                    | 1   | 6     | 1.86     | 2.99    | 0.7    | 1.7        |
| 18       | 6                    | 5   | 11    | 1.98     | 4.01    | 0.72   | 1.91       |
| 19       | 8                    | 3   | 11    | 2.24     | 5.97    | 1.39   | 1.78       |
| 20       | 4                    | 0   | 4     | 2.06     | 3.03    | 0.62   | 1.9        |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %    |
| 9                             | 7   | 16    | 1                        | 5.0  |
| 6                             | 5   | 11    | 2                        | 10.0 |
| 2                             | 1   | 3     | 3                        | 15.0 |
| 4                             | 1   | 5     | 4                        | 20.0 |
| 1                             | 0   | 1     | 5                        | 25.0 |
| 0                             | 1   | 1     | 6                        | 30.0 |
| 0                             | 0   | 0     | 7                        | 35.0 |
| 0                             | 0   | 0     | 8                        | 40.0 |
| 0                             | 2   | 2     | 9                        | 45.0 |
| 0                             | 0   | 0     | 10                       | 50.0 |
| 1                             | 0   | 1     | 11                       | 55.0 |

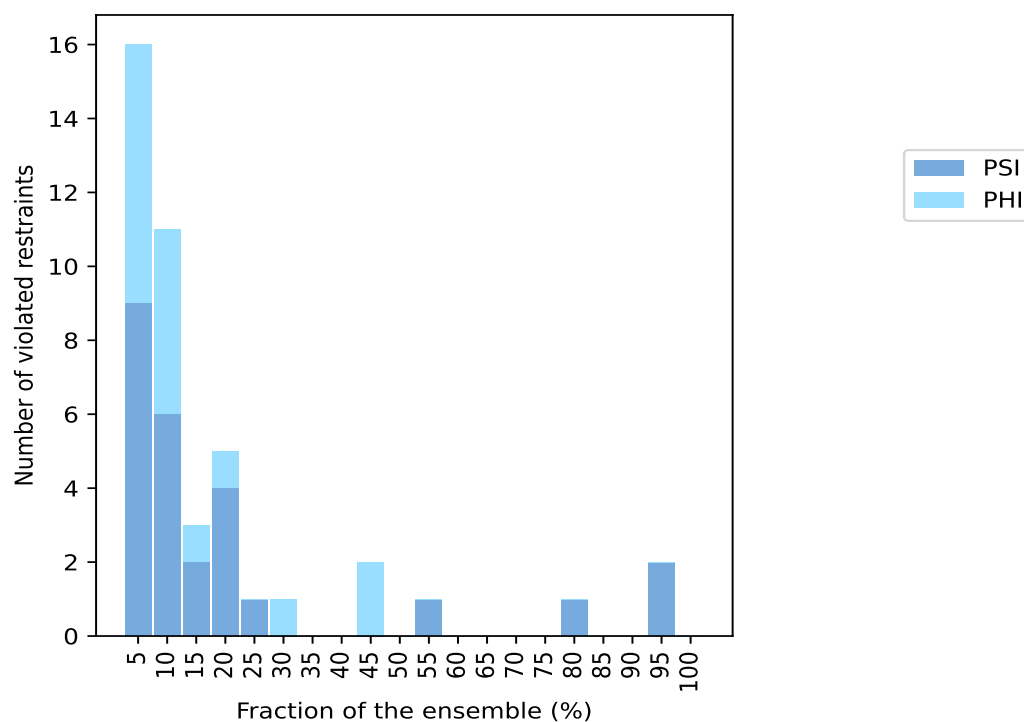
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |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

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

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

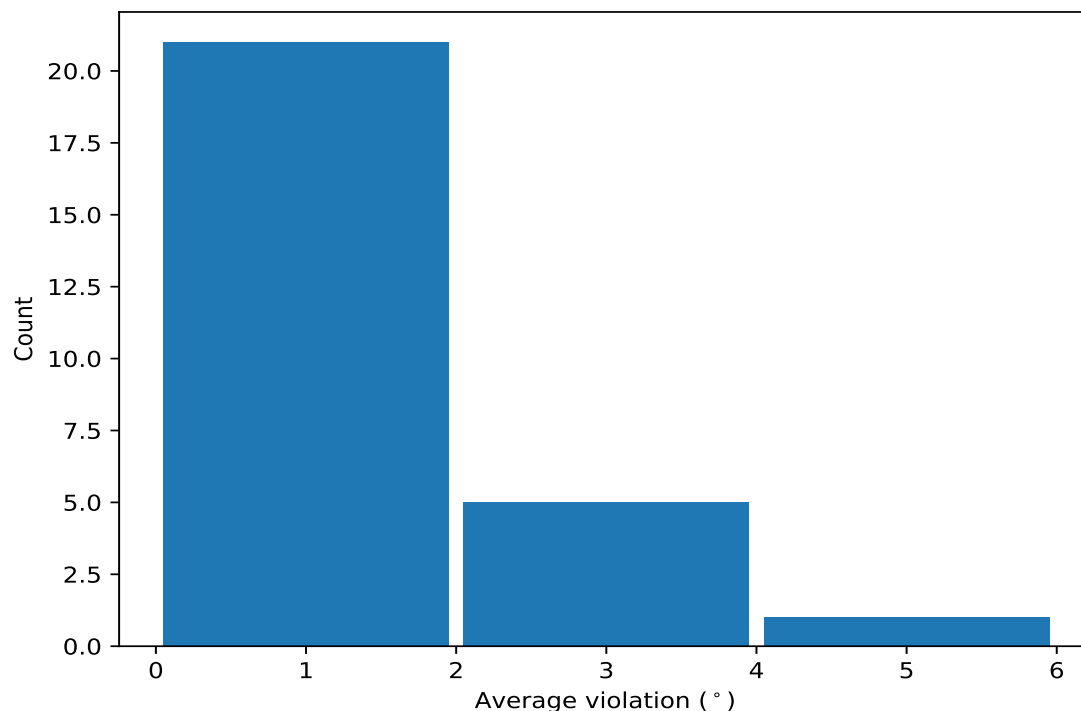


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



#### 10.4.2 Table: Most violated dihedral-angle restraints ⓘ

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 |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 19                  | 3.09 | 0.64            | 3.01   |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 19                  | 2.08 | 0.58            | 1.91   |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 16                  | 1.92 | 0.53            | 1.9    |
| (1,14)  | 1:10:A:THR:N  | 1:10:A:THR:CA  | 1:10:A:THR:C   | 1:11:A:THR:N  | 11                  | 1.65 | 0.58            | 1.56   |
| (1,109) | 1:103:A:LYS:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 9                   | 1.59 | 0.25            | 1.62   |
| (1,105) | 1:101:A:GLU:C | 1:102:A:ILE:N  | 1:102:A:ILE:CA | 1:102:A:ILE:C | 9                   | 1.38 | 0.32            | 1.34   |
| (1,11)  | 1:8:A:GLU:C   | 1:9:A:THR:N    | 1:9:A:THR:CA   | 1:9:A:THR:C   | 6                   | 1.48 | 0.3             | 1.42   |
| (1,30)  | 1:19:A:PHE:N  | 1:19:A:PHE:CA  | 1:19:A:PHE:C   | 1:20:A:LYS:N  | 5                   | 1.44 | 0.25            | 1.25   |
| (1,173) | 1:152:A:LEU:N | 1:152:A:LEU:CA | 1:152:A:LEU:C  | 1:153:A:ALA:N | 4                   | 3.5  | 1.68            | 3.08   |
| (1,172) | 1:151:A:LEU:N | 1:151:A:LEU:CA | 1:151:A:LEU:C  | 1:152:A:LEU:N | 4                   | 2.27 | 0.81            | 2.26   |
| (1,55)  | 1:40:A:SER:N  | 1:40:A:SER:CA  | 1:40:A:SER:C   | 1:41:A:SER:N  | 4                   | 1.72 | 0.55            | 1.62   |
| (1,9)   | 1:7:A:SER:C   | 1:8:A:GLU:N    | 1:8:A:GLU:CA   | 1:8:A:GLU:C   | 4                   | 1.63 | 0.51            | 1.61   |
| (1,10)  | 1:8:A:GLU:N   | 1:8:A:GLU:CA   | 1:8:A:GLU:C    | 1:9:A:THR:N   | 4                   | 1.32 | 0.2             | 1.23   |
| (1,92)  | 1:85:A:LEU:N  | 1:85:A:LEU:CA  | 1:85:A:LEU:C   | 1:86:A:ILE:N  | 3                   | 2.1  | 1.23            | 1.39   |
| (1,120) | 1:113:A:ILE:N | 1:113:A:ILE:CA | 1:113:A:ILE:C  | 1:114:A:LEU:N | 3                   | 1.53 | 0.33            | 1.73   |
| (1,117) | 1:108:A:PRO:C | 1:109:A:ASP:N  | 1:109:A:ASP:CA | 1:109:A:ASP:C | 3                   | 1.47 | 0.25            | 1.58   |
| (1,56)  | 1:42:A:GLU:C  | 1:43:A:ILE:N   | 1:43:A:ILE:CA  | 1:43:A:ILE:C  | 2                   | 5.2  | 1.88            | 5.2    |
| (1,104) | 1:101:A:GLU:N | 1:101:A:GLU:CA | 1:101:A:GLU:C  | 1:102:A:ILE:N | 2                   | 1.6  | 0.59            | 1.6    |
| (1,59)  | 1:44:A:ILE:N  | 1:44:A:ILE:CA  | 1:44:A:ILE:C   | 1:45:A:GLU:N  | 2                   | 1.58 | 0.55            | 1.58   |
| (1,93)  | 1:93:A:GLU:C  | 1:94:A:THR:N   | 1:94:A:THR:CA  | 1:94:A:THR:C  | 2                   | 1.56 | 0.14            | 1.56   |

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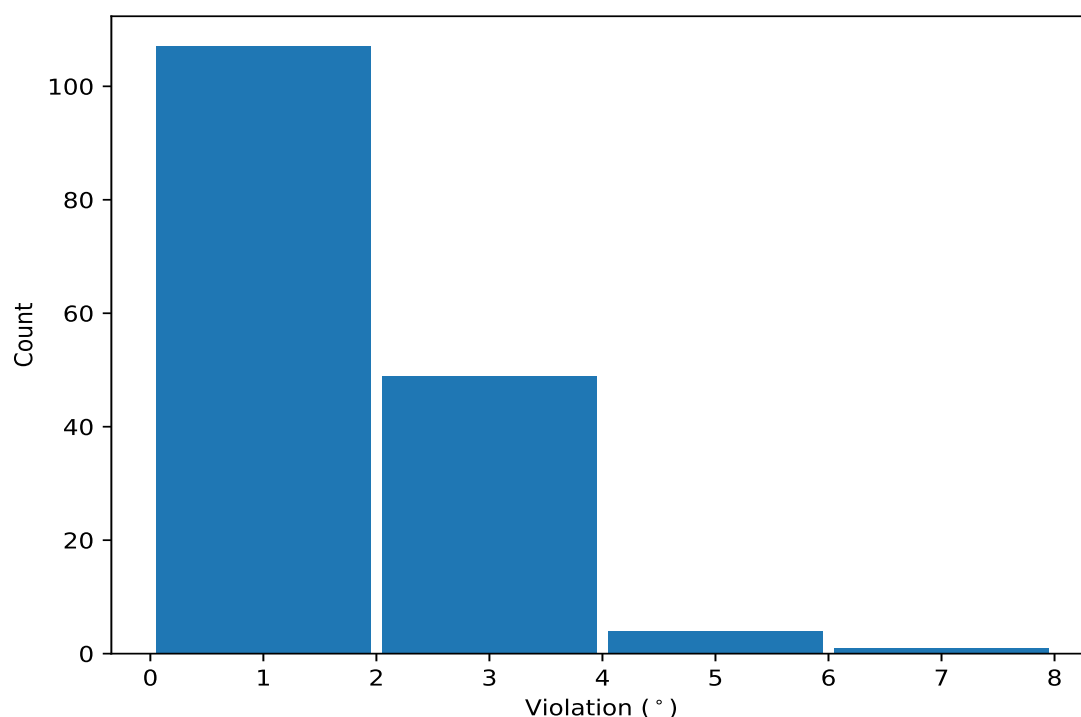
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,68)  | 1:54:A:LYS:C  | 1:55:A:LYS:N   | 1:55:A:LYS:CA  | 1:55:A:LYS:C  | 2                   | 1.54 | 0.09            | 1.54   |
| (1,2)   | 1:4:A:THR:N   | 1:4:A:THR:CA   | 1:4:A:THR:C    | 1:5:A:TYR:N   | 2                   | 1.43 | 0.32            | 1.43   |
| (1,122) | 1:114:A:LEU:N | 1:114:A:LEU:CA | 1:114:A:LEU:C  | 1:115:A:LYS:N | 2                   | 1.41 | 0.36            | 1.41   |
| (1,43)  | 1:31:A:PRO:N  | 1:31:A:PRO:CA  | 1:31:A:PRO:C   | 1:32:A:LYS:N  | 2                   | 1.31 | 0.05            | 1.31   |
| (1,107) | 1:102:A:ILE:C | 1:103:A:LYS:N  | 1:103:A:LYS:CA | 1:103:A:LYS:C | 2                   | 1.11 | 0.06            | 1.11   |
| (1,131) | 1:119:A:LYS:C | 1:120:A:TYR:N  | 1:120:A:TYR:CA | 1:120:A:TYR:C | 2                   | 1.1  | 0.07            | 1.1    |
| (1,132) | 1:120:A:TYR:N | 1:120:A:TYR:CA | 1:120:A:TYR:C  | 1:121:A:HIS:N | 2                   | 1.06 | 0.04            | 1.06   |

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

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

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

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



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

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

| Key    | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,56) | 1:42:A:GLU:C | 1:43:A:ILE:N | 1:43:A:ILE:CA | 1:43:A:ILE:C | 15       | 7.09          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,173) | 1:152:A:LEU:N | 1:152:A:LEU:CA | 1:152:A:LEU:C  | 1:153:A:ALA:N | 19       | 5.97          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 12       | 4.18          |
| (1,173) | 1:152:A:LEU:N | 1:152:A:LEU:CA | 1:152:A:LEU:C  | 1:153:A:ALA:N | 16       | 4.13          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 18       | 4.01          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 2        | 3.95          |
| (1,92)  | 1:85:A:LEU:N  | 1:85:A:LEU:CA  | 1:85:A:LEU:C   | 1:86:A:ILE:N  | 5        | 3.83          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 9        | 3.77          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 1        | 3.71          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 8        | 3.66          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 19       | 3.59          |
| (1,172) | 1:151:A:LEU:N | 1:151:A:LEU:CA | 1:151:A:LEU:C  | 1:152:A:LEU:N | 2        | 3.43          |
| (1,56)  | 1:42:A:GLU:C  | 1:43:A:ILE:N   | 1:43:A:ILE:CA  | 1:43:A:ILE:C  | 10       | 3.32          |
| (1,14)  | 1:10:A:THR:N  | 1:10:A:THR:CA  | 1:10:A:THR:C   | 1:11:A:THR:N  | 4        | 3.26          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 12       | 3.17          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 2        | 3.12          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 20       | 3.03          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 7        | 3.02          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 13       | 3.01          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 17       | 2.99          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 14       | 2.93          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 15       | 2.86          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 15       | 2.83          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 8        | 2.82          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 14       | 2.78          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 4        | 2.67          |
| (1,99)  | 1:98:A:ILE:C  | 1:99:A:ALA:N   | 1:99:A:ALA:CA  | 1:99:A:ALA:C  | 12       | 2.66          |
| (1,55)  | 1:40:A:SER:N  | 1:40:A:SER:CA  | 1:40:A:SER:C   | 1:41:A:SER:N  | 1        | 2.59          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 19       | 2.53          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 13       | 2.52          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 8        | 2.47          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 3        | 2.47          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 18       | 2.45          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 17       | 2.44          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 16       | 2.41          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 10       | 2.39          |
| (1,172) | 1:151:A:LEU:N | 1:151:A:LEU:CA | 1:151:A:LEU:C  | 1:152:A:LEU:N | 19       | 2.36          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 10       | 2.33          |
| (1,9)   | 1:7:A:SER:C   | 1:8:A:GLU:N    | 1:8:A:GLU:CA   | 1:8:A:GLU:C   | 5        | 2.29          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 5        | 2.26          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 19       | 2.22          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 7        | 2.21          |
| (1,104) | 1:101:A:GLU:N | 1:101:A:GLU:CA | 1:101:A:GLU:C  | 1:102:A:ILE:N | 13       | 2.18          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 5        | 2.16          |
| (1,172) | 1:151:A:LEU:N | 1:151:A:LEU:CA | 1:151:A:LEU:C  | 1:152:A:LEU:N | 13       | 2.15          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 20       | 2.14          |
| (1,59)  | 1:44:A:ILE:N  | 1:44:A:ILE:CA  | 1:44:A:ILE:C   | 1:45:A:GLU:N  | 15       | 2.13          |
| (1,90)  | 1:84:A:THR:N  | 1:84:A:THR:CA  | 1:84:A:THR:C   | 1:85:A:LEU:N  | 6        | 2.12          |
| (1,94)  | 1:94:A:THR:N  | 1:94:A:THR:CA  | 1:94:A:THR:C   | 1:95:A:LEU:N  | 2        | 2.11          |
| (1,105) | 1:101:A:GLU:C | 1:102:A:ILE:N  | 1:102:A:ILE:CA | 1:102:A:ILE:C | 17       | 2.07          |
| (1,11)  | 1:8:A:GLU:C   | 1:9:A:THR:N    | 1:9:A:THR:CA   | 1:9:A:THR:C   | 18       | 2.07          |
| (1,173) | 1:152:A:LEU:N | 1:152:A:LEU:CA | 1:152:A:LEU:C  | 1:153:A:ALA:N | 2        | 2.04          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,31)  | 1:20:A:LYS:C  | 1:21:A:ALA:N   | 1:21:A:ALA:CA  | 1:21:A:ALA:C  | 15       | 2.01          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 5        | 2.0           |
| (1,14)  | 1:10:A:THR:N  | 1:10:A:THR:CA  | 1:10:A:THR:C   | 1:11:A:THR:N  | 6        | 1.97          |
| (1,109) | 1:103:A:LYS:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 18       | 1.96          |
| (1,9)   | 1:7:A:SER:C   | 1:8:A:GLU:N    | 1:8:A:GLU:CA   | 1:8:A:GLU:C   | 18       | 1.94          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 13       | 1.93          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 3        | 1.91          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 18       | 1.91          |
| (1,14)  | 1:10:A:THR:N  | 1:10:A:THR:CA  | 1:10:A:THR:C   | 1:11:A:THR:N  | 7        | 1.89          |
| (1,173) | 1:152:A:LEU:N | 1:152:A:LEU:CA | 1:152:A:LEU:C  | 1:153:A:ALA:N | 13       | 1.86          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 11       | 1.86          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 1        | 1.83          |
| (1,109) | 1:103:A:LYS:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 9        | 1.8           |
| (1,120) | 1:113:A:ILE:N | 1:113:A:ILE:CA | 1:113:A:ILE:C  | 1:114:A:LEU:N | 12       | 1.79          |
| (1,109) | 1:103:A:LYS:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 19       | 1.78          |
| (1,30)  | 1:19:A:PHE:N  | 1:19:A:PHE:CA  | 1:19:A:PHE:C   | 1:20:A:LYS:N  | 7        | 1.78          |
| (1,122) | 1:114:A:LEU:N | 1:114:A:LEU:CA | 1:114:A:LEU:C  | 1:115:A:LYS:N | 15       | 1.77          |
| (1,2)   | 1:4:A:THR:N   | 1:4:A:THR:CA   | 1:4:A:THR:C    | 1:5:A:TYR:N   | 10       | 1.75          |
| (1,120) | 1:113:A:ILE:N | 1:113:A:ILE:CA | 1:113:A:ILE:C  | 1:114:A:LEU:N | 18       | 1.73          |
| (1,109) | 1:103:A:LYS:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 1        | 1.73          |
| (1,30)  | 1:19:A:PHE:N  | 1:19:A:PHE:CA  | 1:19:A:PHE:C   | 1:20:A:LYS:N  | 16       | 1.72          |
| (1,117) | 1:108:A:PRO:C | 1:109:A:ASP:N  | 1:109:A:ASP:CA | 1:109:A:ASP:C | 11       | 1.7           |
| (1,93)  | 1:93:A:GLU:C  | 1:94:A:THR:N   | 1:94:A:THR:CA  | 1:94:A:THR:C  | 12       | 1.7           |
| (1,55)  | 1:40:A:SER:N  | 1:40:A:SER:CA  | 1:40:A:SER:C   | 1:41:A:SER:N  | 15       | 1.7           |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 15       | 1.69          |
| (1,14)  | 1:10:A:THR:N  | 1:10:A:THR:CA  | 1:10:A:THR:C   | 1:11:A:THR:N  | 19       | 1.68          |
| (1,10)  | 1:8:A:GLU:N   | 1:8:A:GLU:CA   | 1:8:A:GLU:C    | 1:9:A:THR:N   | 14       | 1.66          |
| (1,105) | 1:101:A:GLU:C | 1:102:A:ILE:N  | 1:102:A:ILE:CA | 1:102:A:ILE:C | 9        | 1.65          |
| (1,14)  | 1:10:A:THR:N  | 1:10:A:THR:CA  | 1:10:A:THR:C   | 1:11:A:THR:N  | 20       | 1.65          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 16       | 1.63          |
| (1,71)  | 1:56:A:ILE:N  | 1:56:A:ILE:CA  | 1:56:A:ILE:C   | 1:57:A:THR:N  | 8        | 1.63          |
| (1,109) | 1:103:A:LYS:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 2        | 1.62          |
| (1,68)  | 1:54:A:LYS:C  | 1:55:A:LYS:N   | 1:55:A:LYS:CA  | 1:55:A:LYS:C  | 14       | 1.62          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 9        | 1.59          |
| (1,117) | 1:108:A:PRO:C | 1:109:A:ASP:N  | 1:109:A:ASP:CA | 1:109:A:ASP:C | 2        | 1.58          |
| (1,11)  | 1:8:A:GLU:C   | 1:9:A:THR:N    | 1:9:A:THR:CA   | 1:9:A:THR:C   | 9        | 1.58          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 2        | 1.56          |
| (1,14)  | 1:10:A:THR:N  | 1:10:A:THR:CA  | 1:10:A:THR:C   | 1:11:A:THR:N  | 18       | 1.56          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 16       | 1.56          |
| (1,55)  | 1:40:A:SER:N  | 1:40:A:SER:CA  | 1:40:A:SER:C   | 1:41:A:SER:N  | 6        | 1.54          |
| (1,109) | 1:103:A:LYS:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 11       | 1.53          |
| (1,36)  | 1:27:A:ASP:N  | 1:27:A:ASP:CA  | 1:27:A:ASP:C   | 1:28:A:ASN:N  | 7        | 1.53          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 4        | 1.53          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 14       | 1.51          |
| (1,105) | 1:101:A:GLU:C | 1:102:A:ILE:N  | 1:102:A:ILE:CA | 1:102:A:ILE:C | 5        | 1.51          |
| (1,135) | 1:129:A:LYS:C | 1:130:A:GLU:N  | 1:130:A:GLU:CA | 1:130:A:GLU:C | 18       | 1.5           |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 6        | 1.48          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 3        | 1.47          |
| (1,130) | 1:119:A:LYS:N | 1:119:A:LYS:CA | 1:119:A:LYS:C  | 1:120:A:TYR:N | 10       | 1.46          |
| (1,11)  | 1:8:A:GLU:C   | 1:9:A:THR:N    | 1:9:A:THR:CA   | 1:9:A:THR:C   | 4        | 1.46          |
| (1,68)  | 1:54:A:LYS:C  | 1:55:A:LYS:N   | 1:55:A:LYS:CA  | 1:55:A:LYS:C  | 18       | 1.45          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 20       | 1.42          |
| (1,93)  | 1:93:A:GLU:C  | 1:94:A:THR:N   | 1:94:A:THR:CA  | 1:94:A:THR:C  | 10       | 1.42          |
| (1,109) | 1:103:A:LYS:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 10       | 1.4           |
| (1,105) | 1:101:A:GLU:C | 1:102:A:ILE:N  | 1:102:A:ILE:CA | 1:102:A:ILE:C | 15       | 1.4           |
| (1,92)  | 1:85:A:LEU:N  | 1:85:A:LEU:CA  | 1:85:A:LEU:C   | 1:86:A:ILE:N  | 4        | 1.39          |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 11       | 1.39          |
| (1,11)  | 1:8:A:GLU:C   | 1:9:A:THR:N    | 1:9:A:THR:CA   | 1:9:A:THR:C   | 12       | 1.39          |
| (1,109) | 1:103:A:LYS:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 13       | 1.38          |
| (1,43)  | 1:31:A:PRO:N  | 1:31:A:PRO:CA  | 1:31:A:PRO:C   | 1:32:A:LYS:N  | 10       | 1.35          |
| (1,105) | 1:101:A:GLU:C | 1:102:A:ILE:N  | 1:102:A:ILE:CA | 1:102:A:ILE:C | 19       | 1.34          |
| (1,84)  | 1:81:A:TYR:N  | 1:81:A:TYR:CA  | 1:81:A:TYR:C   | 1:82:A:ALA:N  | 17       | 1.33          |
| (1,14)  | 1:10:A:THR:N  | 1:10:A:THR:CA  | 1:10:A:THR:C   | 1:11:A:THR:N  | 8        | 1.31          |
| (1,105) | 1:101:A:GLU:C | 1:102:A:ILE:N  | 1:102:A:ILE:CA | 1:102:A:ILE:C | 12       | 1.3           |
| (1,12)  | 1:9:A:THR:N   | 1:9:A:THR:CA   | 1:9:A:THR:C    | 1:10:A:THR:N  | 7        | 1.3           |
| (1,10)  | 1:8:A:GLU:N   | 1:8:A:GLU:CA   | 1:8:A:GLU:C    | 1:9:A:THR:N   | 16       | 1.28          |
| (1,9)   | 1:7:A:SER:C   | 1:8:A:GLU:N    | 1:8:A:GLU:CA   | 1:8:A:GLU:C   | 8        | 1.28          |
| (1,98)  | 1:98:A:ILE:N  | 1:98:A:ILE:CA  | 1:98:A:ILE:C   | 1:99:A:ALA:N  | 12       | 1.27          |
| (1,14)  | 1:10:A:THR:N  | 1:10:A:THR:CA  | 1:10:A:THR:C   | 1:11:A:THR:N  | 3        | 1.27          |
| (1,43)  | 1:31:A:PRO:N  | 1:31:A:PRO:CA  | 1:31:A:PRO:C   | 1:32:A:LYS:N  | 15       | 1.26          |
| (1,14)  | 1:10:A:THR:N  | 1:10:A:THR:CA  | 1:10:A:THR:C   | 1:11:A:THR:N  | 13       | 1.26          |
| (1,30)  | 1:19:A:PHE:N  | 1:19:A:PHE:CA  | 1:19:A:PHE:C   | 1:20:A:LYS:N  | 18       | 1.25          |
| (1,30)  | 1:19:A:PHE:N  | 1:19:A:PHE:CA  | 1:19:A:PHE:C   | 1:20:A:LYS:N  | 5        | 1.24          |
| (1,30)  | 1:19:A:PHE:N  | 1:19:A:PHE:CA  | 1:19:A:PHE:C   | 1:20:A:LYS:N  | 12       | 1.23          |
| (1,106) | 1:102:A:ILE:N | 1:102:A:ILE:CA | 1:102:A:ILE:C  | 1:103:A:LYS:N | 6        | 1.2           |
| (1,14)  | 1:10:A:THR:N  | 1:10:A:THR:CA  | 1:10:A:THR:C   | 1:11:A:THR:N  | 2        | 1.2           |
| (1,126) | 1:117:A:THR:N | 1:117:A:THR:CA | 1:117:A:THR:C  | 1:118:A:SER:N | 2        | 1.19          |
| (1,11)  | 1:8:A:GLU:C   | 1:9:A:THR:N    | 1:9:A:THR:CA   | 1:9:A:THR:C   | 2        | 1.19          |
| (1,6)   | 1:6:A:GLU:N   | 1:6:A:GLU:CA   | 1:6:A:GLU:C    | 1:7:A:SER:N   | 17       | 1.19          |
| (1,131) | 1:119:A:LYS:C | 1:120:A:TYR:N  | 1:120:A:TYR:CA | 1:120:A:TYR:C | 4        | 1.18          |
| (1,11)  | 1:8:A:GLU:C   | 1:9:A:THR:N    | 1:9:A:THR:CA   | 1:9:A:THR:C   | 3        | 1.18          |
| (1,10)  | 1:8:A:GLU:N   | 1:8:A:GLU:CA   | 1:8:A:GLU:C    | 1:9:A:THR:N   | 13       | 1.18          |
| (1,107) | 1:102:A:ILE:C | 1:103:A:LYS:N  | 1:103:A:LYS:CA | 1:103:A:LYS:C | 9        | 1.17          |
| (1,10)  | 1:8:A:GLU:N   | 1:8:A:GLU:CA   | 1:8:A:GLU:C    | 1:9:A:THR:N   | 8        | 1.17          |
| (1,123) | 1:115:A:LYS:C | 1:116:A:SER:N  | 1:116:A:SER:CA | 1:116:A:SER:C | 7        | 1.16          |
| (1,172) | 1:151:A:LEU:N | 1:151:A:LEU:CA | 1:151:A:LEU:C  | 1:152:A:LEU:N | 16       | 1.14          |
| (1,177) | 1:155:A:PRO:C | 1:156:A:ALA:N  | 1:156:A:ALA:CA | 1:156:A:ALA:C | 4        | 1.13          |
| (1,117) | 1:108:A:PRO:C | 1:109:A:ASP:N  | 1:109:A:ASP:CA | 1:109:A:ASP:C | 15       | 1.13          |
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 17       | 1.12          |
| (1,14)  | 1:10:A:THR:N  | 1:10:A:THR:CA  | 1:10:A:THR:C   | 1:11:A:THR:N  | 14       | 1.12          |
| (1,105) | 1:101:A:GLU:C | 1:102:A:ILE:N  | 1:102:A:ILE:CA | 1:102:A:ILE:C | 2        | 1.11          |
| (1,27)  | 1:17:A:ARG:C  | 1:18:A:LEU:N   | 1:18:A:LEU:CA  | 1:18:A:LEU:C  | 10       | 1.11          |
| (1,2)   | 1:4:A:THR:N   | 1:4:A:THR:CA   | 1:4:A:THR:C    | 1:5:A:TYR:N   | 19       | 1.11          |
| (1,132) | 1:120:A:TYR:N | 1:120:A:TYR:CA | 1:120:A:TYR:C  | 1:121:A:HIS:N | 10       | 1.09          |
| (1,109) | 1:103:A:LYS:C | 1:104:A:LEU:N  | 1:104:A:LEU:CA | 1:104:A:LEU:C | 5        | 1.09          |
| (1,92)  | 1:85:A:LEU:N  | 1:85:A:LEU:CA  | 1:85:A:LEU:C   | 1:86:A:ILE:N  | 2        | 1.09          |
| (1,120) | 1:113:A:ILE:N | 1:113:A:ILE:CA | 1:113:A:ILE:C  | 1:114:A:LEU:N | 5        | 1.07          |
| (1,89)  | 1:83:A:CYS:C  | 1:84:A:THR:N   | 1:84:A:THR:CA  | 1:84:A:THR:C  | 5        | 1.07          |
| (1,55)  | 1:40:A:SER:N  | 1:40:A:SER:CA  | 1:40:A:SER:C   | 1:41:A:SER:N  | 9        | 1.06          |
| (1,122) | 1:114:A:LEU:N | 1:114:A:LEU:CA | 1:114:A:LEU:C  | 1:115:A:LYS:N | 3        | 1.05          |
| (1,107) | 1:102:A:ILE:C | 1:103:A:LYS:N  | 1:103:A:LYS:CA | 1:103:A:LYS:C | 10       | 1.05          |
| (1,131) | 1:119:A:LYS:C | 1:120:A:TYR:N  | 1:120:A:TYR:CA | 1:120:A:TYR:C | 19       | 1.03          |

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*Continued from previous page...*

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,124) | 1:116:A:SER:N | 1:116:A:SER:CA | 1:116:A:SER:C  | 1:117:A:THR:N | 6        | 1.03          |
| (1,105) | 1:101:A:GLU:C | 1:102:A:ILE:N  | 1:102:A:ILE:CA | 1:102:A:ILE:C | 6        | 1.03          |
| (1,132) | 1:120:A:TYR:N | 1:120:A:TYR:CA | 1:120:A:TYR:C  | 1:121:A:HIS:N | 19       | 1.02          |
| (1,59)  | 1:44:A:ILE:N  | 1:44:A:ILE:CA  | 1:44:A:ILE:C   | 1:45:A:GLU:N  | 10       | 1.02          |
| (1,105) | 1:101:A:GLU:C | 1:102:A:ILE:N  | 1:102:A:ILE:CA | 1:102:A:ILE:C | 7        | 1.01          |
| (1,104) | 1:101:A:GLU:N | 1:101:A:GLU:CA | 1:101:A:GLU:C  | 1:102:A:ILE:N | 16       | 1.01          |
| (1,9)   | 1:7:A:SER:C   | 1:8:A:GLU:N    | 1:8:A:GLU:CA   | 1:8:A:GLU:C   | 7        | 1.01          |