



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:15 PM UTC

PDB ID : 2M5C / pdb\_00002m5c  
BMRB ID : 19047  
Title : Solution Structure of the Bacillus cereus Metallo-Beta-Lactamase BcII  
Authors : Karsisiotis, A.I.; Damblon, C.F.; Roberts, G.C.K.  
Deposited on : 2013-02-20

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

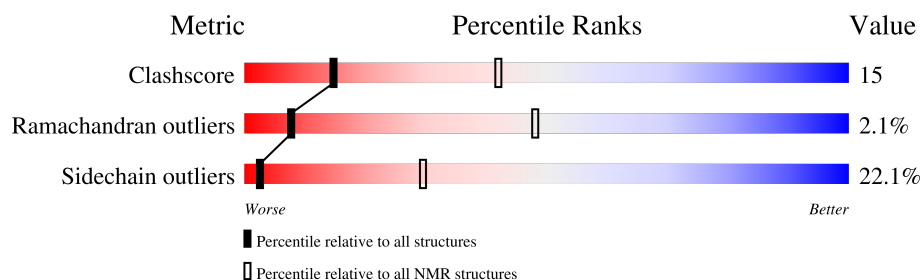
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 84%.

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     | 227    | <div> <div></div> <div>53%</div> <div>32%</div> <div>5%</div> <div>10%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:8-A:32, A:39-A:173,<br>A:184-A:227 (204) | 0.27              | 7            |

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

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

The models can be grouped into 4 clusters and 5 single-model clusters were found.

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

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

There are 2 unique types of molecules in this entry. The entry contains 3590 atoms, of which 1830 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Beta-lactamase 2.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|-------|
| 1   | A     | 227      | Total | C    | H    | N   | O   | S | 0     |
|     |       |          | 3588  | 1113 | 1830 | 304 | 338 | 3 |       |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

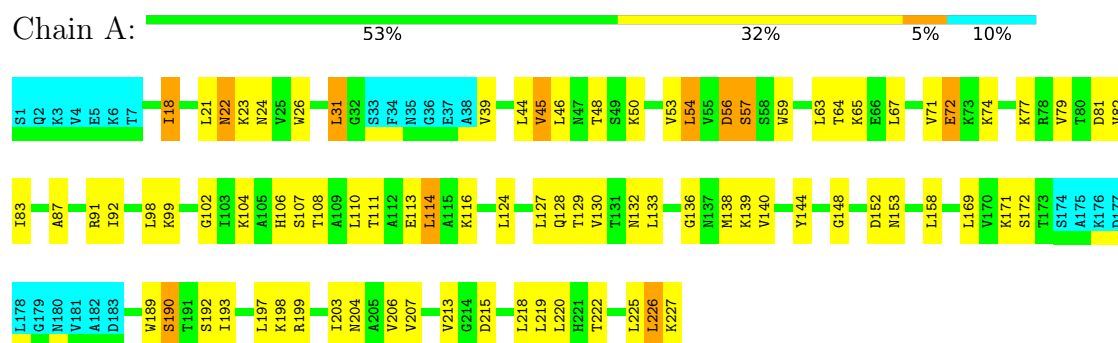
| Mol | Chain | Residues | Atoms |    |
|-----|-------|----------|-------|----|
| 2   | A     | 2        | Total | Zn |
|     |       |          | 2     | 2  |

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

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

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

- Molecule 1: Beta-lactamase 2

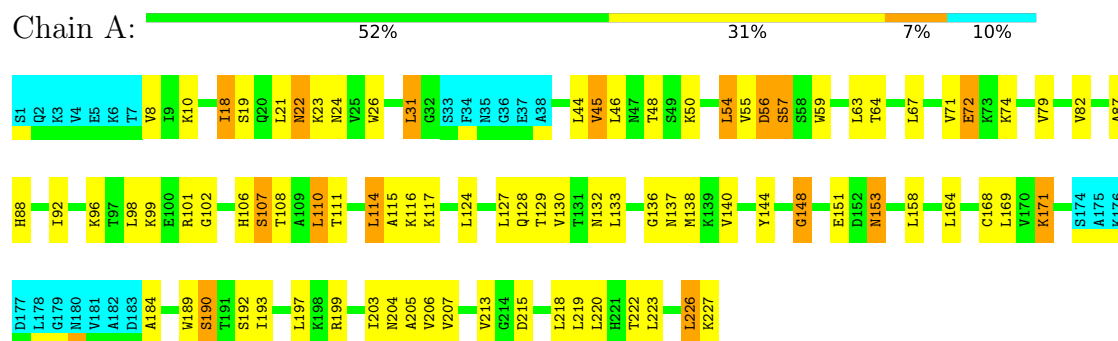


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

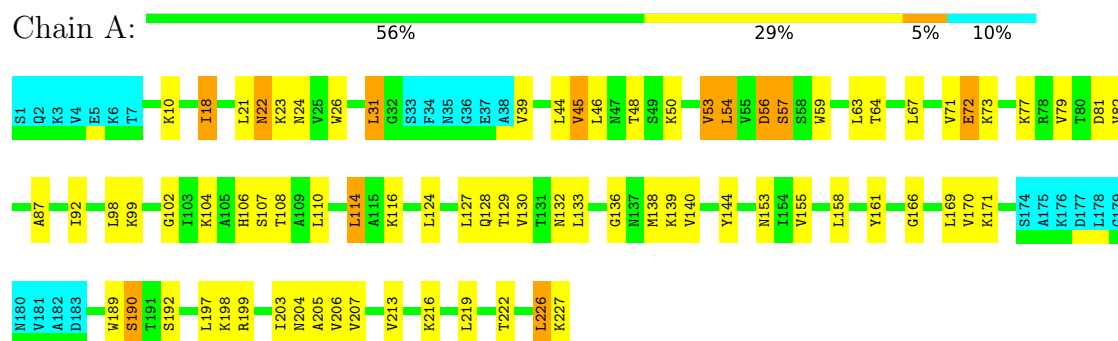
#### 4.2.1 Score per residue for model 1

- Molecule 1: Beta-lactamase 2



## 4.2.2 Score per residue for model 2

### • Molecule 1: Beta-lactamase 2



## 4.2.3 Score per residue for model 3

### • Molecule 1: Beta-lactamase 2



## 4.2.4 Score per residue for model 4

### • Molecule 1: Beta-lactamase 2



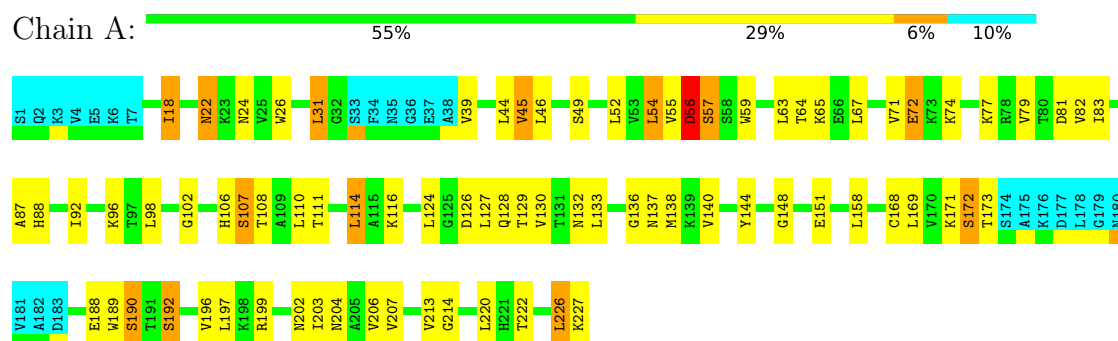
### 4.2.5 Score per residue for model 5

- Molecule 1: Beta-lactamase 2



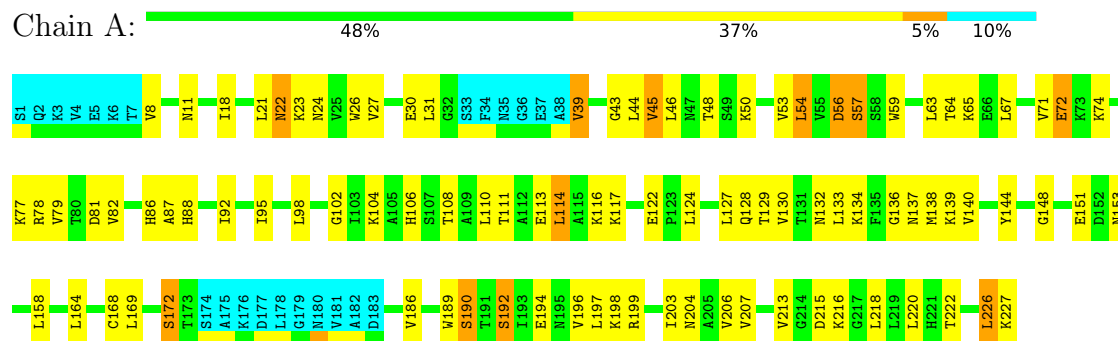
### 4.2.6 Score per residue for model 6

- Molecule 1: Beta-lactamase 2



### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Beta-lactamase 2



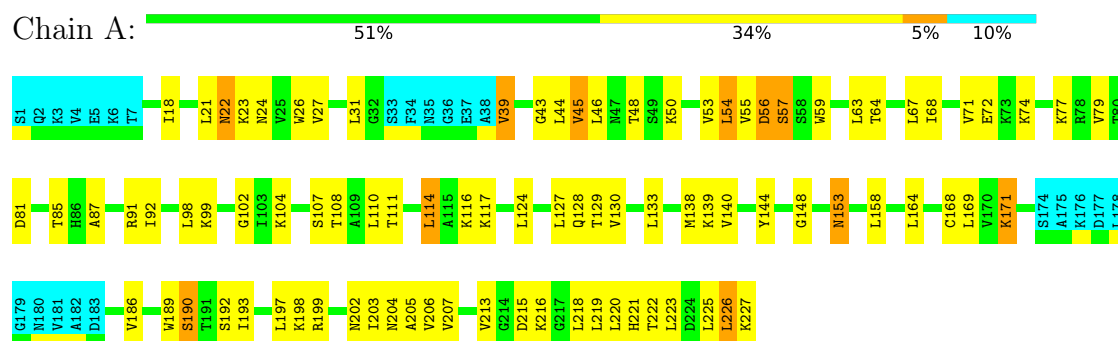
### 4.2.8 Score per residue for model 8

- Molecule 1: Beta-lactamase 2



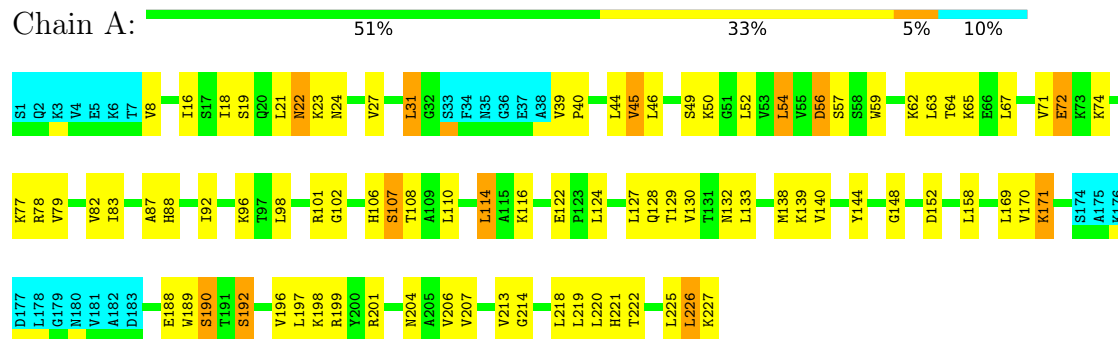
### 4.2.9 Score per residue for model 9

- Molecule 1: Beta-lactamase 2



### 4.2.10 Score per residue for model 10

- Molecule 1: Beta-lactamase 2



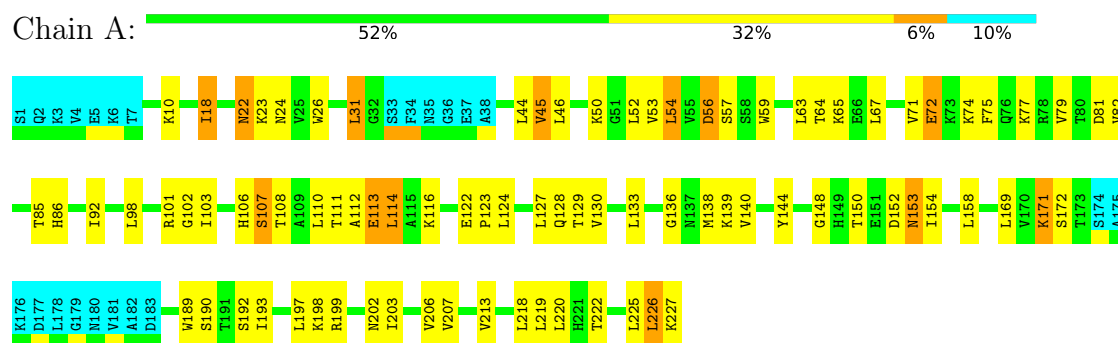
## 4.2.11 Score per residue for model 11

- Molecule 1: Beta-lactamase 2



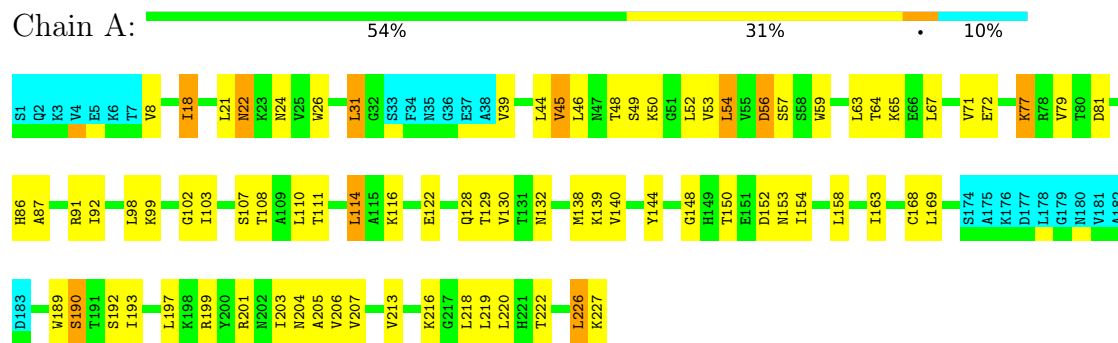
## 4.2.12 Score per residue for model 12

- Molecule 1: Beta-lactamase 2



## 4.2.13 Score per residue for model 13

- Molecule 1: Beta-lactamase 2



### 4.2.14 Score per residue for model 14

- Molecule 1: Beta-lactamase 2



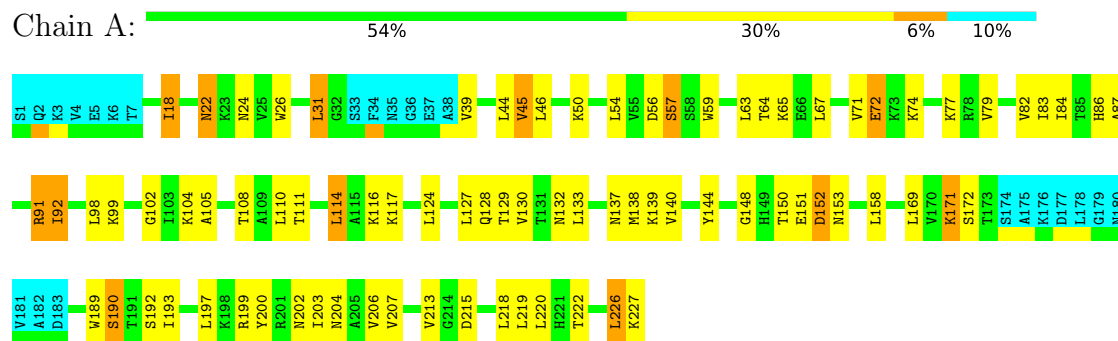
### 4.2.15 Score per residue for model 15

- Molecule 1: Beta-lactamase 2



### 4.2.16 Score per residue for model 16

- Molecule 1: Beta-lactamase 2



## 4.2.17 Score per residue for model 17

- Molecule 1: Beta-lactamase 2



## 4.2.20 Score per residue for model 20

### • Molecule 1: Beta-lactamase 2



## 5 Refinement protocol and experimental data overview

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

Of the 100 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 |
|---------------|--------------------|---------|
| CYANA         | structure solution |         |
| CYANA         | refinement         |         |
| CANDID        | structure solution |         |

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               | 2              |
| Total number of shifts                       | 4075           |
| Number of shifts mapped to atoms             | 4075           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 84%            |

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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     | 1591  | 1666     | 1638     | 49±5    |
| All | All   | 31860 | 33320    | 32760    | 980     |

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 15.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:207:VAL:HG22 | 1:A:213:VAL:HG12 | 0.91     | 1.41        | 16     | 13    |
| 1:A:84:ILE:HD11  | 1:A:105:ALA:HB1  | 0.88     | 1.42        | 15     | 5     |
| 1:A:207:VAL:HG22 | 1:A:213:VAL:HG22 | 0.88     | 1.45        | 1      | 5     |
| 1:A:21:LEU:HD21  | 1:A:213:VAL:HG21 | 0.86     | 1.48        | 5      | 5     |
| 1:A:222:THR:HG22 | 1:A:226:LEU:HD23 | 0.83     | 1.49        | 11     | 15    |
| 1:A:21:LEU:HD21  | 1:A:213:VAL:HG11 | 0.81     | 1.49        | 19     | 7     |
| 1:A:140:VAL:HG22 | 1:A:158:LEU:HD21 | 0.81     | 1.54        | 2      | 17    |
| 1:A:84:ILE:HD12  | 1:A:91:ARG:CZ    | 0.80     | 2.07        | 15     | 5     |
| 1:A:84:ILE:HG23  | 1:A:91:ARG:NE    | 0.78     | 1.94        | 17     | 5     |
| 1:A:87:ALA:HB2   | 1:A:114:LEU:HD13 | 0.76     | 1.56        | 20     | 16    |
| 1:A:129:THR:HG22 | 1:A:130:VAL:HG23 | 0.75     | 1.57        | 17     | 20    |
| 1:A:46:LEU:HD21  | 1:A:158:LEU:HD11 | 0.72     | 1.59        | 17     | 12    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:190:SER:CB   | 1:A:226:LEU:HD11 | 0.65     | 2.21        | 17     | 20    |
| 1:A:30:GLU:CD    | 1:A:67:LEU:HD22  | 0.64     | 2.18        | 20     | 3     |
| 1:A:104:LYS:HE2  | 1:A:124:LEU:HD21 | 0.64     | 1.69        | 19     | 7     |
| 1:A:222:THR:HG22 | 1:A:226:LEU:CD2  | 0.64     | 2.23        | 18     | 17    |
| 1:A:87:ALA:CB    | 1:A:114:LEU:HD13 | 0.64     | 2.23        | 18     | 15    |
| 1:A:104:LYS:CE   | 1:A:124:LEU:HD21 | 0.63     | 2.24        | 19     | 5     |
| 1:A:190:SER:OG   | 1:A:223:LEU:HD23 | 0.63     | 1.93        | 17     | 3     |
| 1:A:221:HIS:CE1  | 1:A:225:LEU:HD11 | 0.63     | 2.28        | 9      | 4     |
| 1:A:207:VAL:HG22 | 1:A:213:VAL:HB   | 0.62     | 1.71        | 19     | 2     |
| 1:A:205:ALA:HB1  | 1:A:213:VAL:CG1  | 0.62     | 2.24        | 13     | 5     |
| 1:A:110:LEU:HD23 | 1:A:152:ASP:OD1  | 0.62     | 1.94        | 12     | 5     |
| 1:A:169:LEU:HD12 | 1:A:189:TRP:NE1  | 0.62     | 2.10        | 12     | 19    |
| 1:A:68:ILE:HG12  | 1:A:79:VAL:HG11  | 0.62     | 1.71        | 9      | 1     |
| 1:A:57:SER:HB3   | 1:A:98:LEU:HD11  | 0.62     | 1.72        | 15     | 16    |
| 1:A:44:LEU:HD21  | 1:A:158:LEU:HD12 | 0.61     | 1.72        | 20     | 13    |
| 1:A:190:SER:HB2  | 1:A:226:LEU:HD11 | 0.61     | 1.71        | 4      | 3     |
| 1:A:156:VAL:O    | 1:A:164:LEU:HD12 | 0.61     | 1.96        | 17     | 3     |
| 1:A:18:ILE:HG22  | 1:A:26:TRP:HB3   | 0.61     | 1.73        | 2      | 19    |
| 1:A:84:ILE:O     | 1:A:154:ILE:HD11 | 0.60     | 1.96        | 15     | 3     |
| 1:A:110:LEU:HD23 | 1:A:152:ASP:OD2  | 0.60     | 1.97        | 11     | 2     |
| 1:A:127:LEU:CD2  | 1:A:133:LEU:HD21 | 0.60     | 2.27        | 3      | 11    |
| 1:A:110:LEU:HD12 | 1:A:113:GLU:HG2  | 0.60     | 1.74        | 18     | 2     |
| 1:A:83:ILE:CD1   | 1:A:140:VAL:HG11 | 0.60     | 2.26        | 14     | 10    |
| 1:A:205:ALA:HB1  | 1:A:213:VAL:CG2  | 0.60     | 2.26        | 19     | 2     |
| 1:A:111:THR:HA   | 1:A:114:LEU:HD11 | 0.59     | 1.74        | 15     | 17    |
| 1:A:46:LEU:HB3   | 1:A:138:MET:HE3  | 0.59     | 1.74        | 5      | 20    |
| 1:A:72:GLU:OE2   | 1:A:79:VAL:HG23  | 0.59     | 1.97        | 12     | 10    |
| 1:A:57:SER:CB    | 1:A:98:LEU:HD11  | 0.59     | 2.27        | 17     | 19    |
| 1:A:190:SER:HB3  | 1:A:226:LEU:HD11 | 0.59     | 1.72        | 11     | 17    |
| 1:A:127:LEU:HD22 | 1:A:133:LEU:HD21 | 0.59     | 1.74        | 8      | 6     |
| 1:A:46:LEU:CD2   | 1:A:158:LEU:HD11 | 0.59     | 2.27        | 6      | 5     |
| 1:A:206:VAL:HB   | 1:A:218:LEU:HD12 | 0.58     | 1.75        | 19     | 17    |
| 1:A:72:GLU:OE1   | 1:A:79:VAL:HG23  | 0.58     | 1.98        | 4      | 5     |
| 1:A:153:ASN:OD1  | 1:A:169:LEU:HD13 | 0.58     | 1.98        | 9      | 8     |
| 1:A:140:VAL:HG22 | 1:A:158:LEU:CD2  | 0.58     | 2.27        | 2      | 15    |
| 1:A:110:LEU:HD22 | 1:A:113:GLU:OE1  | 0.58     | 1.98        | 15     | 1     |
| 1:A:45:VAL:HG13  | 1:A:54:LEU:CD2   | 0.58     | 2.29        | 2      | 20    |
| 1:A:207:VAL:HG22 | 1:A:213:VAL:CG1  | 0.58     | 2.28        | 7      | 13    |
| 1:A:104:LYS:HD3  | 1:A:124:LEU:HD21 | 0.58     | 1.73        | 15     | 1     |
| 1:A:131:THR:HG22 | 1:A:142:THR:OG1  | 0.58     | 1.99        | 5      | 1     |
| 1:A:203:ILE:HG21 | 1:A:206:VAL:HG22 | 0.57     | 1.76        | 3      | 16    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:152:ASP:O    | 1:A:154:ILE:HG23 | 0.57     | 1.98        | 8      | 3     |
| 1:A:54:LEU:O     | 1:A:82:VAL:HG13  | 0.57     | 1.99        | 5      | 14    |
| 1:A:129:THR:HG23 | 1:A:144:TYR:HB3  | 0.57     | 1.77        | 4      | 20    |
| 1:A:57:SER:OG    | 1:A:98:LEU:HD11  | 0.57     | 1.99        | 2      | 5     |
| 1:A:203:ILE:HG21 | 1:A:206:VAL:CG2  | 0.57     | 2.29        | 4      | 13    |
| 1:A:44:LEU:HD21  | 1:A:158:LEU:HD11 | 0.56     | 1.78        | 5      | 3     |
| 1:A:171:LYS:HG2  | 1:A:222:THR:HG23 | 0.56     | 1.78        | 16     | 5     |
| 1:A:110:LEU:HD12 | 1:A:152:ASP:HB3  | 0.56     | 1.76        | 8      | 1     |
| 1:A:84:ILE:CD1   | 1:A:105:ALA:HB1  | 0.55     | 2.29        | 17     | 4     |
| 1:A:84:ILE:HD11  | 1:A:105:ALA:CB   | 0.55     | 2.29        | 17     | 4     |
| 1:A:55:VAL:HG12  | 1:A:56:ASP:OD1   | 0.55     | 2.02        | 6      | 3     |
| 1:A:207:VAL:CG2  | 1:A:213:VAL:HG12 | 0.55     | 2.29        | 8      | 8     |
| 1:A:207:VAL:HG22 | 1:A:213:VAL:CG2  | 0.55     | 2.27        | 13     | 5     |
| 1:A:98:LEU:HA    | 1:A:103:ILE:HD13 | 0.54     | 1.78        | 13     | 5     |
| 1:A:81:ASP:N     | 1:A:103:ILE:HG23 | 0.54     | 2.17        | 14     | 3     |
| 1:A:192:SER:O    | 1:A:196:VAL:HG23 | 0.54     | 2.02        | 10     | 5     |
| 1:A:226:LEU:HD12 | 1:A:226:LEU:O    | 0.54     | 2.03        | 12     | 19    |
| 1:A:106:HIS:HA   | 1:A:124:LEU:HD12 | 0.54     | 1.79        | 5      | 12    |
| 1:A:53:VAL:HG13  | 1:A:81:ASP:CB    | 0.54     | 2.32        | 14     | 2     |
| 1:A:44:LEU:HD21  | 1:A:158:LEU:CD1  | 0.54     | 2.33        | 5      | 9     |
| 1:A:31:LEU:HD12  | 1:A:40:PRO:HB3   | 0.54     | 1.80        | 14     | 3     |
| 1:A:107:SER:CA   | 1:A:127:LEU:HD12 | 0.54     | 2.33        | 6      | 9     |
| 1:A:83:ILE:HD13  | 1:A:140:VAL:HG11 | 0.53     | 1.79        | 14     | 6     |
| 1:A:59:TRP:HB2   | 1:A:63:LEU:HD12  | 0.53     | 1.80        | 5      | 20    |
| 1:A:164:LEU:HD22 | 1:A:203:ILE:HD13 | 0.53     | 1.79        | 15     | 8     |
| 1:A:45:VAL:HG22  | 1:A:54:LEU:HD23  | 0.52     | 1.80        | 16     | 7     |
| 1:A:171:LYS:HE3  | 1:A:225:LEU:HD11 | 0.52     | 1.80        | 11     | 1     |
| 1:A:205:ALA:HB1  | 1:A:213:VAL:HG11 | 0.52     | 1.79        | 5      | 3     |
| 1:A:52:LEU:HB3   | 1:A:79:VAL:HG22  | 0.52     | 1.81        | 15     | 7     |
| 1:A:21:LEU:HG    | 1:A:27:VAL:HG23  | 0.52     | 1.80        | 10     | 2     |
| 1:A:53:VAL:HG13  | 1:A:81:ASP:O     | 0.52     | 2.05        | 20     | 6     |
| 1:A:104:LYS:HE3  | 1:A:124:LEU:HD21 | 0.52     | 1.80        | 7      | 3     |
| 1:A:56:ASP:OD2   | 1:A:85:THR:HG23  | 0.51     | 2.05        | 14     | 1     |
| 1:A:45:VAL:HG13  | 1:A:54:LEU:HD23  | 0.51     | 1.82        | 5      | 12    |
| 1:A:222:THR:C    | 1:A:226:LEU:HD23 | 0.51     | 2.31        | 13     | 9     |
| 1:A:91:ARG:HH22  | 1:A:95:ILE:HD12  | 0.51     | 1.65        | 20     | 2     |
| 1:A:193:ILE:HG21 | 1:A:219:LEU:O    | 0.51     | 2.06        | 8      | 11    |
| 1:A:144:TYR:CD1  | 1:A:154:ILE:HG22 | 0.50     | 2.41        | 12     | 3     |
| 1:A:107:SER:HA   | 1:A:127:LEU:HD12 | 0.50     | 1.84        | 6      | 4     |
| 1:A:164:LEU:HD22 | 1:A:203:ILE:CD1  | 0.50     | 2.37        | 14     | 8     |
| 1:A:54:LEU:HD11  | 1:A:79:VAL:HG21  | 0.50     | 1.83        | 20     | 6     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:67:LEU:O     | 1:A:71:VAL:HG22  | 0.49     | 2.06        | 5      | 18    |
| 1:A:53:VAL:HG13  | 1:A:81:ASP:HB2   | 0.49     | 1.84        | 9      | 1     |
| 1:A:52:LEU:HD11  | 1:A:75:PHE:HB2   | 0.49     | 1.83        | 14     | 6     |
| 1:A:27:VAL:HG13  | 1:A:43:GLY:O     | 0.49     | 2.08        | 14     | 5     |
| 1:A:16:ILE:HD13  | 1:A:67:LEU:HB2   | 0.49     | 1.85        | 10     | 2     |
| 1:A:110:LEU:HD23 | 1:A:152:ASP:CG   | 0.49     | 2.32        | 12     | 2     |
| 1:A:104:LYS:HB3  | 1:A:124:LEU:HD11 | 0.49     | 1.83        | 8      | 6     |
| 1:A:91:ARG:HH21  | 1:A:92:ILE:HG22  | 0.49     | 1.65        | 16     | 5     |
| 1:A:57:SER:OG    | 1:A:98:LEU:HD21  | 0.49     | 2.07        | 16     | 2     |
| 1:A:92:ILE:O     | 1:A:95:ILE:HG22  | 0.49     | 2.08        | 18     | 1     |
| 1:A:171:LYS:HD3  | 1:A:222:THR:HG23 | 0.49     | 1.84        | 10     | 1     |
| 1:A:222:THR:O    | 1:A:226:LEU:HD23 | 0.48     | 2.08        | 7      | 2     |
| 1:A:107:SER:OG   | 1:A:111:THR:HG21 | 0.48     | 2.08        | 6      | 2     |
| 1:A:27:VAL:HG21  | 1:A:213:VAL:CG2  | 0.48     | 2.39        | 9      | 1     |
| 1:A:170:VAL:HG13 | 1:A:219:LEU:HA   | 0.48     | 1.85        | 10     | 7     |
| 1:A:21:LEU:HD13  | 1:A:163:ILE:HD13 | 0.48     | 1.84        | 19     | 3     |
| 1:A:67:LEU:O     | 1:A:67:LEU:HD12  | 0.47     | 2.09        | 17     | 5     |
| 1:A:22:ASN:N     | 1:A:22:ASN:ND2   | 0.47     | 2.63        | 18     | 20    |
| 1:A:148:GLY:O    | 1:A:184:ALA:HB1  | 0.47     | 2.09        | 3      | 4     |
| 1:A:106:HIS:CA   | 1:A:124:LEU:HD12 | 0.47     | 2.39        | 5      | 1     |
| 1:A:54:LEU:O     | 1:A:82:VAL:HG22  | 0.47     | 2.09        | 19     | 4     |
| 1:A:84:ILE:HG23  | 1:A:91:ARG:HE    | 0.47     | 1.68        | 20     | 1     |
| 1:A:111:THR:HG23 | 1:A:152:ASP:OD1  | 0.46     | 2.11        | 15     | 2     |
| 1:A:86:HIS:HB2   | 1:A:150:THR:HG21 | 0.46     | 1.87        | 12     | 8     |
| 1:A:91:ARG:NH2   | 1:A:95:ILE:HD12  | 0.46     | 2.25        | 20     | 1     |
| 1:A:110:LEU:HD12 | 1:A:113:GLU:CG   | 0.46     | 2.41        | 12     | 1     |
| 1:A:106:HIS:CG   | 1:A:124:LEU:HD12 | 0.46     | 2.46        | 6      | 2     |
| 1:A:171:LYS:CE   | 1:A:225:LEU:HD11 | 0.46     | 2.40        | 11     | 1     |
| 1:A:207:VAL:CG2  | 1:A:213:VAL:HG22 | 0.45     | 2.34        | 15     | 3     |
| 1:A:207:VAL:HG13 | 1:A:213:VAL:HG12 | 0.45     | 1.87        | 10     | 3     |
| 1:A:110:LEU:HD22 | 1:A:113:GLU:CD   | 0.45     | 2.35        | 4      | 2     |
| 1:A:127:LEU:HD21 | 1:A:133:LEU:HD21 | 0.45     | 1.88        | 2      | 2     |
| 1:A:55:VAL:HG11  | 1:A:165:VAL:HG11 | 0.45     | 1.88        | 15     | 1     |
| 1:A:52:LEU:HD13  | 1:A:77:LYS:HB2   | 0.45     | 1.89        | 13     | 1     |
| 1:A:30:GLU:OE2   | 1:A:67:LEU:HD22  | 0.45     | 2.12        | 19     | 1     |
| 1:A:15:THR:HG23  | 1:A:31:LEU:HB3   | 0.45     | 1.89        | 14     | 2     |
| 1:A:114:LEU:HD23 | 1:A:151:GLU:HB3  | 0.45     | 1.89        | 1      | 4     |
| 1:A:112:ALA:HB2  | 1:A:123:PRO:HG2  | 0.45     | 1.89        | 18     | 4     |
| 1:A:110:LEU:HD21 | 1:A:151:GLU:HG2  | 0.44     | 1.88        | 7      | 2     |
| 1:A:169:LEU:HD12 | 1:A:189:TRP:HE1  | 0.44     | 1.72        | 18     | 3     |
| 1:A:55:VAL:HG12  | 1:A:56:ASP:CG    | 0.44     | 2.37        | 1      | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:54:LEU:CD1   | 1:A:79:VAL:HG21  | 0.43     | 2.44        | 2      | 4     |
| 1:A:197:LEU:C    | 1:A:197:LEU:HD12 | 0.43     | 2.38        | 20     | 17    |
| 1:A:46:LEU:HD21  | 1:A:158:LEU:HD21 | 0.43     | 1.89        | 4      | 1     |
| 1:A:172:SER:O    | 1:A:173:THR:C    | 0.43     | 2.62        | 11     | 1     |
| 1:A:200:TYR:O    | 1:A:203:ILE:HD11 | 0.43     | 2.14        | 16     | 1     |
| 1:A:95:ILE:HG12  | 1:A:121:GLU:CG   | 0.42     | 2.44        | 18     | 1     |
| 1:A:171:LYS:HG3  | 1:A:225:LEU:HD12 | 0.42     | 1.91        | 3      | 2     |
| 1:A:53:VAL:HG13  | 1:A:81:ASP:C     | 0.42     | 2.39        | 4      | 2     |
| 1:A:203:ILE:HG21 | 1:A:206:VAL:HG23 | 0.42     | 1.91        | 4      | 1     |
| 1:A:18:ILE:CD1   | 1:A:71:VAL:HG12  | 0.42     | 2.45        | 7      | 3     |
| 1:A:67:LEU:O     | 1:A:71:VAL:HG13  | 0.42     | 2.15        | 20     | 2     |
| 1:A:108:THR:HG22 | 1:A:127:LEU:C    | 0.42     | 2.40        | 4      | 1     |
| 1:A:52:LEU:HD11  | 1:A:75:PHE:CB    | 0.42     | 2.44        | 12     | 2     |
| 1:A:114:LEU:HD12 | 1:A:115:ALA:N    | 0.41     | 2.30        | 1      | 1     |
| 1:A:152:ASP:O    | 1:A:152:ASP:CG   | 0.41     | 2.60        | 8      | 1     |
| 1:A:190:SER:OG   | 1:A:226:LEU:HD11 | 0.41     | 2.15        | 5      | 1     |
| 1:A:16:ILE:HG21  | 1:A:67:LEU:HD13  | 0.41     | 1.91        | 17     | 1     |
| 1:A:39:VAL:HG12  | 1:A:59:TRP:CZ2   | 0.41     | 2.50        | 19     | 1     |
| 1:A:155:VAL:HG12 | 1:A:166:GLY:HA2  | 0.41     | 1.92        | 2      | 1     |
| 1:A:83:ILE:C     | 1:A:84:ILE:HD13  | 0.41     | 2.40        | 20     | 1     |
| 1:A:111:THR:HG23 | 1:A:152:ASP:OD2  | 0.40     | 2.16        | 19     | 1     |
| 1:A:197:LEU:HD12 | 1:A:197:LEU:C    | 0.40     | 2.41        | 14     | 3     |
| 1:A:220:LEU:HA   | 1:A:223:LEU:HD12 | 0.40     | 1.93        | 14     | 1     |
| 1:A:139:LYS:O    | 1:A:158:LEU:HD23 | 0.40     | 2.16        | 9      | 1     |
| 1:A:53:VAL:HG22  | 1:A:81:ASP:HB2   | 0.40     | 1.94        | 14     | 1     |
| 1:A:83:ILE:HG21  | 1:A:156:VAL:HG22 | 0.40     | 1.91        | 20     | 1     |
| 1:A:81:ASP:O     | 1:A:82:VAL:HG23  | 0.40     | 2.16        | 14     | 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     | 203/227 (89%)   | 175±3 (86±1%) | 24±3 (12±1%) | 4±1 (2±1%) | 8           | 48 |
| All | All   | 4060/4540 (89%) | 3499 (86%)    | 476 (12%)    | 85 (2%)    | 8           | 48 |

All 11 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     | 102 | GLY  | 19             |
| 1   | A     | 148 | GLY  | 17             |
| 1   | A     | 56  | ASP  | 15             |
| 1   | A     | 136 | GLY  | 12             |
| 1   | A     | 8   | VAL  | 8              |
| 1   | A     | 202 | ASN  | 6              |
| 1   | A     | 214 | GLY  | 3              |
| 1   | A     | 171 | LYS  | 2              |
| 1   | A     | 57  | SER  | 1              |
| 1   | A     | 22  | ASN  | 1              |
| 1   | A     | 11  | ASN  | 1              |

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

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

| Mol | Chain | Analysed        | Rotameric     | Outliers     | Percentiles |    |
|-----|-------|-----------------|---------------|--------------|-------------|----|
| 1   | A     | 178/196 (91%)   | 139±4 (78±2%) | 39±4 (22±2%) | 2           | 29 |
| All | All   | 3560/3920 (91%) | 2772 (78%)    | 788 (22%)    | 2           | 29 |

All 76 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     | 22  | ASN  | 20             |
| 1   | A     | 24  | ASN  | 20             |
| 1   | A     | 45  | VAL  | 20             |
| 1   | A     | 64  | THR  | 20             |
| 1   | A     | 92  | ILE  | 20             |
| 1   | A     | 108 | THR  | 20             |
| 1   | A     | 114 | LEU  | 20             |
| 1   | A     | 116 | LYS  | 20             |
| 1   | A     | 128 | GLN  | 20             |
| 1   | A     | 192 | SER  | 20             |
| 1   | A     | 226 | LEU  | 20             |
| 1   | A     | 72  | GLU  | 19             |
| 1   | A     | 204 | ASN  | 19             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 50  | LYS  | 18             |
| 1   | A     | 153 | ASN  | 18             |
| 1   | A     | 190 | SER  | 18             |
| 1   | A     | 227 | LYS  | 17             |
| 1   | A     | 77  | LYS  | 17             |
| 1   | A     | 54  | LEU  | 16             |
| 1   | A     | 132 | ASN  | 16             |
| 1   | A     | 199 | ARG  | 16             |
| 1   | A     | 220 | LEU  | 16             |
| 1   | A     | 56  | ASP  | 16             |
| 1   | A     | 31  | LEU  | 15             |
| 1   | A     | 23  | LYS  | 14             |
| 1   | A     | 48  | THR  | 14             |
| 1   | A     | 39  | VAL  | 14             |
| 1   | A     | 18  | ILE  | 13             |
| 1   | A     | 74  | LYS  | 13             |
| 1   | A     | 99  | LYS  | 13             |
| 1   | A     | 215 | ASP  | 13             |
| 1   | A     | 139 | LYS  | 13             |
| 1   | A     | 107 | SER  | 12             |
| 1   | A     | 110 | LEU  | 12             |
| 1   | A     | 198 | LYS  | 12             |
| 1   | A     | 65  | LYS  | 11             |
| 1   | A     | 88  | HIS  | 10             |
| 1   | A     | 168 | CYS  | 10             |
| 1   | A     | 216 | LYS  | 10             |
| 1   | A     | 96  | LYS  | 9              |
| 1   | A     | 117 | LYS  | 9              |
| 1   | A     | 137 | ASN  | 9              |
| 1   | A     | 171 | LYS  | 9              |
| 1   | A     | 57  | SER  | 9              |
| 1   | A     | 49  | SER  | 8              |
| 1   | A     | 122 | GLU  | 8              |
| 1   | A     | 10  | LYS  | 7              |
| 1   | A     | 101 | ARG  | 7              |
| 1   | A     | 73  | LYS  | 7              |
| 1   | A     | 113 | GLU  | 7              |
| 1   | A     | 172 | SER  | 7              |
| 1   | A     | 91  | ARG  | 7              |
| 1   | A     | 53  | VAL  | 6              |
| 1   | A     | 90  | ASP  | 5              |
| 1   | A     | 223 | LEU  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 224 | ASP  | 4              |
| 1   | A     | 78  | ARG  | 4              |
| 1   | A     | 134 | LYS  | 4              |
| 1   | A     | 81  | ASP  | 3              |
| 1   | A     | 152 | ASP  | 3              |
| 1   | A     | 201 | ARG  | 3              |
| 1   | A     | 19  | SER  | 2              |
| 1   | A     | 161 | TYR  | 2              |
| 1   | A     | 41  | SER  | 2              |
| 1   | A     | 86  | HIS  | 2              |
| 1   | A     | 173 | THR  | 2              |
| 1   | A     | 188 | GLU  | 2              |
| 1   | A     | 194 | GLU  | 2              |
| 1   | A     | 85  | THR  | 2              |
| 1   | A     | 62  | LYS  | 2              |
| 1   | A     | 154 | ILE  | 1              |
| 1   | A     | 212 | GLU  | 1              |
| 1   | A     | 126 | ASP  | 1              |
| 1   | A     | 95  | ILE  | 1              |
| 1   | A     | 121 | GLU  | 1              |
| 1   | A     | 151 | GLU  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

## 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 84% for the well-defined parts and 83% 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                  | 2293 |
| Number of shifts mapped to atoms        | 2293 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 15   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 202      | $-0.63 \pm 0.09$                | Should be checked          |
| $^{13}\text{C}_\beta$  | 202      | $-0.16 \pm 0.15$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 0        | —                               | None (insufficient data)   |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 75%, i.e. 2111 atoms were assigned a chemical shift out of a possible 2807. 0 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 596/1028 (58%)  | 412/421 (98%)  | 184/408 (45%)   | 0/199 (0%)      |
| Sidechain | 1395/1602 (87%) | 970/1045 (93%) | 425/504 (84%)   | 0/53 (0%)       |

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|          | Total           | <sup>1</sup> H  | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|-----------------|-----------------|-----------------|
| Aromatic | 120/177 (68%)   | 71/87 (82%)     | 49/74 (66%)     | 0/16 (0%)       |
| Overall  | 2111/2807 (75%) | 1453/1553 (94%) | 658/986 (67%)   | 0/268 (0%)      |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 2286 atoms were assigned a chemical shift out of a possible 3082. 0 out of 48 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H  | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone  | 655/1145 (57%)  | 453/469 (97%)   | 202/454 (44%)   | 0/222 (0%)      |
| Sidechain | 1503/1750 (86%) | 1046/1139 (92%) | 457/552 (83%)   | 0/59 (0%)       |
| Aromatic  | 128/187 (68%)   | 76/92 (83%)     | 52/79 (66%)     | 0/16 (0%)       |
| Overall   | 2286/3082 (74%) | 1575/1700 (93%) | 711/1085 (66%)  | 0/297 (0%)      |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

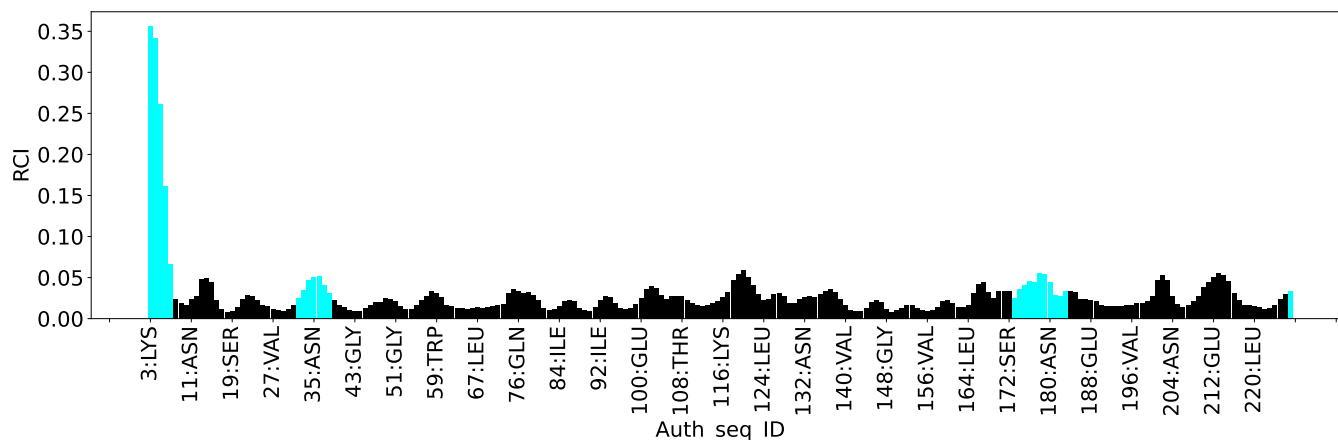
| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 108 | THR  | HG1  | 6.69       | 0.08 – 2.19         | 26.3    |
| 1       | A     | 80  | THR  | HG1  | 6.26       | 0.08 – 2.19         | 24.3    |
| 1       | A     | 48  | THR  | HG1  | 5.65       | 0.08 – 2.19         | 21.4    |
| 1       | A     | 222 | THR  | HG1  | 5.32       | 0.08 – 2.19         | 19.8    |
| 1       | A     | 29  | THR  | HG1  | 4.78       | 0.08 – 2.19         | 17.2    |
| 1       | A     | 200 | TYR  | CD2  | 116.27     | 125.28 – 140.14     | -11.1   |
| 1       | A     | 90  | ASP  | HB3  | 0.40       | 1.32 – 4.00         | -8.4    |
| 1       | A     | 20  | GLN  | HB3  | -0.07      | 0.71 – 3.33         | -8.0    |
| 1       | A     | 199 | ARG  | HD2  | 1.35       | 1.97 – 4.26         | -7.7    |
| 1       | A     | 199 | ARG  | HD3  | 1.23       | 1.81 – 4.39         | -7.3    |
| 1       | A     | 199 | ARG  | HG3  | -0.25      | 0.15 – 2.94         | -6.4    |
| 1       | A     | 147 | LYS  | HD3  | 0.28       | 0.54 – 2.65         | -6.3    |
| 1       | A     | 90  | ASP  | HA   | 2.75       | 3.04 – 6.12         | -5.9    |
| 1       | A     | 32  | GLY  | HA3  | 1.88       | 2.08 – 5.71         | -5.6    |
| 1       | A     | 75  | PHE  | HZ   | 4.82       | 4.94 – 9.06         | -5.3    |

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-

defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



## 7.2 Chemical shift list 2

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

### 7.2.1 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                  | 1782 |
| Number of shifts mapped to atoms        | 1782 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 12   |

### 7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action         |
|------------------------|----------|---------------------------------|--------------------------|
| $^{13}\text{C}_\alpha$ | 0        | —                               | None (insufficient data) |
| $^{13}\text{C}_\beta$  | 0        | —                               | None (insufficient data) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data) |

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| Nucleus         | # values | Correction $\pm$ precision, ppm | Suggested action           |
|-----------------|----------|---------------------------------|----------------------------|
| $^{15}\text{N}$ | 211      | 0.50 $\pm$ 0.25                 | None needed ( $< 0.5$ ppm) |

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 58%, i.e. 1635 atoms were assigned a chemical shift out of a possible 2807. 0 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$    | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone  | 607/1028 (59%)  | 414/421 (98%)   | 0/408 (0%)      | 193/199 (97%)   |
| Sidechain | 974/1602 (61%)  | 957/1045 (92%)  | 0/504 (0%)      | 17/53 (32%)     |
| Aromatic  | 54/177 (31%)    | 50/87 (57%)     | 0/74 (0%)       | 4/16 (25%)      |
| Overall   | 1635/2807 (58%) | 1421/1553 (92%) | 0/986 (0%)      | 214/268 (80%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 58%, i.e. 1775 atoms were assigned a chemical shift out of a possible 3082. 0 out of 48 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$    | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone  | 665/1145 (58%)  | 454/469 (97%)   | 0/454 (0%)      | 211/222 (95%)   |
| Sidechain | 1054/1750 (60%) | 1034/1139 (91%) | 0/552 (0%)      | 20/59 (34%)     |
| Aromatic  | 56/187 (30%)    | 52/92 (57%)     | 0/79 (0%)       | 4/16 (25%)      |
| Overall   | 1775/3082 (58%) | 1540/1700 (91%) | 0/1085 (0%)     | 235/297 (79%)   |

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

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

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 2       | A     | 108 | THR  | HG1  | 6.72       | 0.08 – 2.19         | 26.4    |
| 2       | A     | 80  | THR  | HG1  | 6.28       | 0.08 – 2.19         | 24.4    |
| 2       | A     | 48  | THR  | HG1  | 5.66       | 0.08 – 2.19         | 21.4    |
| 2       | A     | 222 | THR  | HG1  | 5.32       | 0.08 – 2.19         | 19.8    |
| 2       | A     | 29  | THR  | HG1  | 4.77       | 0.08 – 2.19         | 17.2    |
| 2       | A     | 90  | ASP  | HB3  | 0.39       | 1.32 – 4.00         | -8.5    |
| 2       | A     | 20  | GLN  | HB3  | -0.03      | 0.71 – 3.33         | -7.8    |
| 2       | A     | 199 | ARG  | HD3  | 1.22       | 1.81 – 4.39         | -7.3    |
| 2       | A     | 199 | ARG  | HG3  | -0.25      | 0.15 – 2.94         | -6.5    |

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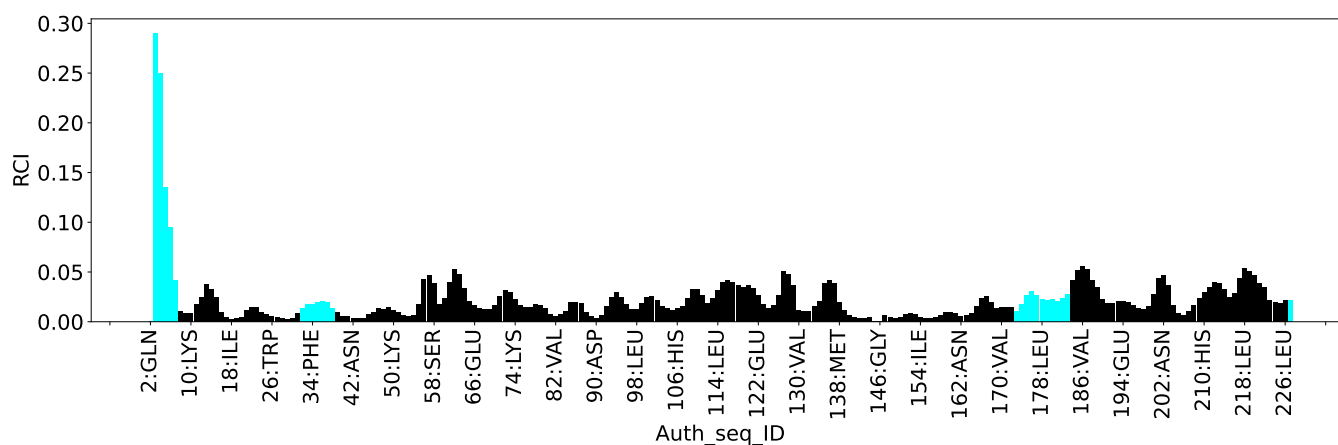
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| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 2       | A     | 147 | LYS  | HD3  | 0.26       | 0.54 – 2.65         | -6.3    |
| 2       | A     | 90  | ASP  | HA   | 2.75       | 3.04 – 6.12         | -5.9    |
| 2       | A     | 32  | GLY  | HA3  | 1.86       | 2.08 – 5.71         | -5.6    |

### 7.2.5 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                                | 6749  |
| Intra-residue ( $ i-j =0$ )                              | 1215  |
| Sequential ( $ i-j =1$ )                                 | 1555  |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 1216  |
| Long range ( $ i-j \geq 5$ )                             | 2753  |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 29.5  |
| Number of long range restraints per residue <sup>1</sup> | 12.0  |

<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)  | 22.1                                   | 0.2     |
| 0.2-0.5 (Medium) | 3.2                                    | 0.47    |
| >0.5 (Large)     | None                                   | None    |

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

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

## 9 Distance violation analysis

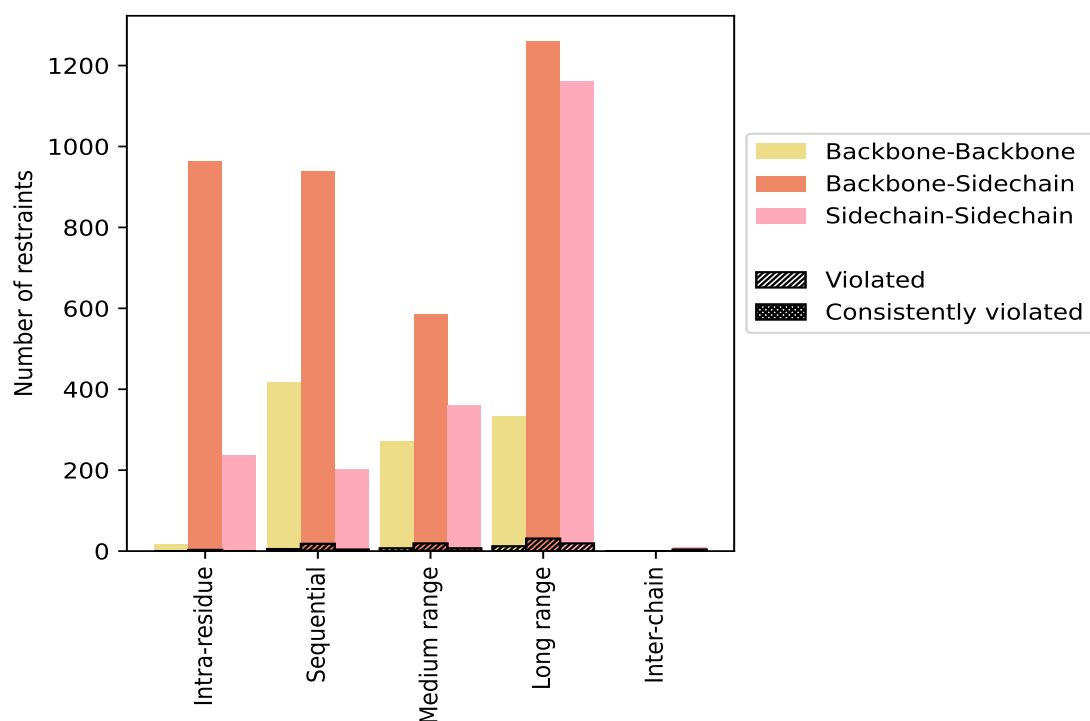
### 9.1 Summary of distance violations

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

| Restrains type                                             | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                     |                     | Consistently Violated <sup>4</sup> |                     |                     |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|---------------------|---------------------|------------------------------------|---------------------|---------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>      | % <sup>1</sup>      | Count                              | % <sup>2</sup>      | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">1215</a> | <a href="#">18.0</a>  | <a href="#">3</a>     | <a href="#">0.2</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 16                   | 0.2                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 962                  | 14.3                  | 3                     | 0.3                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 237                  | 3.5                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">1555</a> | <a href="#">23.0</a>  | <a href="#">26</a>    | <a href="#">1.7</a> | <a href="#">0.4</a> | <a href="#">1</a>                  | <a href="#">0.1</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 417                  | 6.2                   | 5                     | 1.2                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 938                  | 13.9                  | 18                    | 1.9                 | 0.3                 | 1                                  | 0.1                 | 0.0                 |
| Sidechain-Sidechain                                        | 200                  | 3.0                   | 3                     | 1.5                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">1216</a> | <a href="#">18.0</a>  | <a href="#">33</a>    | <a href="#">2.7</a> | <a href="#">0.5</a> | <a href="#">2</a>                  | <a href="#">0.2</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 270                  | 4.0                   | 7                     | 2.6                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 585                  | 8.7                   | 19                    | 3.2                 | 0.3                 | 1                                  | 0.2                 | 0.0                 |
| Sidechain-Sidechain                                        | 361                  | 5.3                   | 7                     | 1.9                 | 0.1                 | 1                                  | 0.3                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">2753</a> | <a href="#">40.8</a>  | <a href="#">62</a>    | <a href="#">2.3</a> | <a href="#">0.9</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 333                  | 4.9                   | 12                    | 3.6                 | 0.2                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 1260                 | 18.7                  | 31                    | 2.5                 | 0.5                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 1160                 | 17.2                  | 19                    | 1.6                 | 0.3                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| 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                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">6749</a> | <a href="#">100.0</a> | <a href="#">129</a>   | <a href="#">1.9</a> | <a href="#">1.9</a> | <a href="#">5</a>                  | <a href="#">0.1</a> | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 1036                 | 15.4                  | 24                    | 2.3                 | 0.4                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 3745                 | 55.5                  | 71                    | 1.9                 | 1.1                 | 2                                  | 0.1                 | 0.0                 |
| Sidechain-Sidechain                                        | 1968                 | 29.2                  | 34                    | 1.7                 | 0.5                 | 3                                  | 0.2                 | 0.0                 |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 0                    | 2               | 4               | 6               | 2               | 14    | 0.15     | 0.22    | 0.03                | 0.14       |
| 2        | 0                    | 6               | 5               | 8               | 3               | 22    | 0.15     | 0.22    | 0.04                | 0.14       |
| 3        | 1                    | 4               | 5               | 7               | 3               | 20    | 0.15     | 0.21    | 0.03                | 0.15       |
| 4        | 1                    | 4               | 5               | 9               | 2               | 21    | 0.15     | 0.21    | 0.03                | 0.14       |
| 5        | 0                    | 5               | 6               | 12              | 2               | 25    | 0.14     | 0.23    | 0.04                | 0.13       |
| 6        | 2                    | 8               | 4               | 9               | 3               | 26    | 0.16     | 0.25    | 0.04                | 0.16       |
| 7        | 1                    | 4               | 7               | 13              | 4               | 29    | 0.14     | 0.23    | 0.04                | 0.13       |
| 8        | 1                    | 6               | 5               | 8               | 1               | 21    | 0.14     | 0.22    | 0.04                | 0.14       |
| 9        | 0                    | 5               | 5               | 14              | 2               | 26    | 0.16     | 0.34    | 0.06                | 0.15       |
| 10       | 1                    | 6               | 6               | 9               | 3               | 25    | 0.16     | 0.36    | 0.06                | 0.15       |

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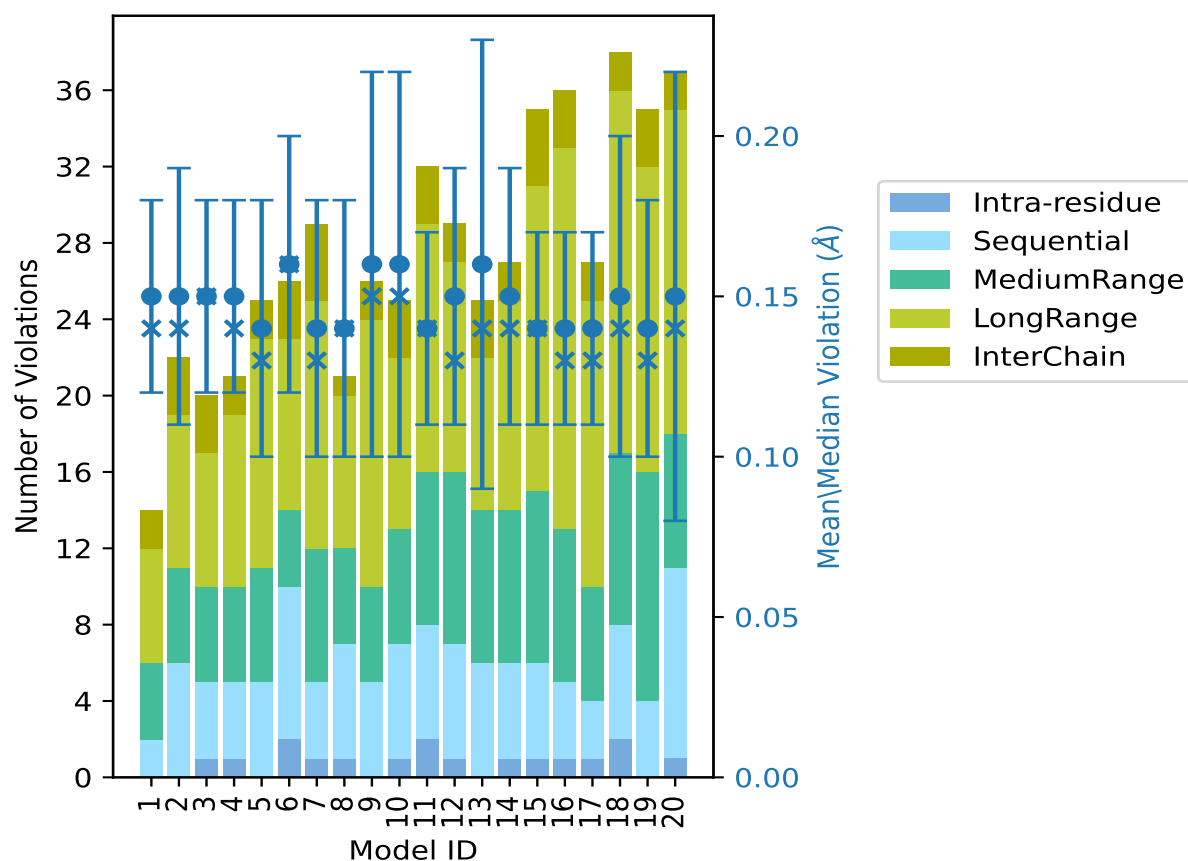
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 2                    | 6               | 8               | 13              | 3               | 32    | 0.14     | 0.21    | 0.03                | 0.14       |
| 12       | 1                    | 6               | 9               | 11              | 2               | 29    | 0.15     | 0.26    | 0.04                | 0.13       |
| 13       | 0                    | 6               | 8               | 8               | 3               | 25    | 0.16     | 0.46    | 0.07                | 0.14       |
| 14       | 1                    | 5               | 8               | 11              | 2               | 27    | 0.15     | 0.25    | 0.04                | 0.14       |
| 15       | 1                    | 5               | 9               | 16              | 4               | 35    | 0.14     | 0.23    | 0.03                | 0.14       |
| 16       | 1                    | 4               | 8               | 20              | 3               | 36    | 0.14     | 0.21    | 0.03                | 0.13       |
| 17       | 1                    | 3               | 6               | 15              | 2               | 27    | 0.14     | 0.22    | 0.03                | 0.13       |
| 18       | 2                    | 6               | 9               | 19              | 2               | 38    | 0.15     | 0.38    | 0.05                | 0.14       |
| 19       | 0                    | 4               | 12              | 16              | 3               | 35    | 0.14     | 0.25    | 0.04                | 0.13       |
| 20       | 1                    | 10              | 7               | 17              | 2               | 37    | 0.15     | 0.47    | 0.07                | 0.14       |

<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

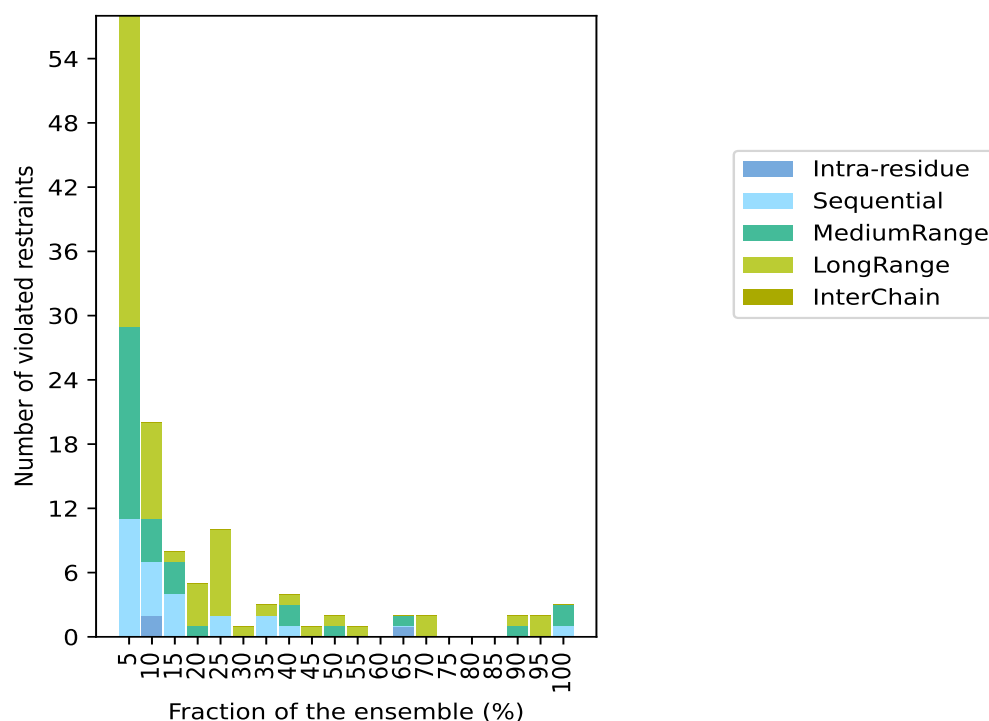
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 6615(IR:1212, SQ:1529, MR:1183, LR:2691, IC:0) restraints 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>       | %     |
| 0                             | 11              | 18              | 29              | 0               | 58    | 1                        | 5.0   |
| 2                             | 5               | 4               | 9               | 0               | 20    | 2                        | 10.0  |
| 0                             | 4               | 3               | 1               | 0               | 8     | 3                        | 15.0  |
| 0                             | 0               | 1               | 4               | 0               | 5     | 4                        | 20.0  |
| 0                             | 2               | 0               | 8               | 0               | 10    | 5                        | 25.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 6                        | 30.0  |
| 0                             | 2               | 0               | 1               | 0               | 3     | 7                        | 35.0  |
| 0                             | 1               | 2               | 1               | 0               | 4     | 8                        | 40.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 9                        | 45.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 10                       | 50.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 11                       | 55.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 12                       | 60.0  |
| 1                             | 0               | 1               | 0               | 0               | 2     | 13                       | 65.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 14                       | 70.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 15                       | 75.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 16                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 85.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 18                       | 90.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 19                       | 95.0  |
| 0                             | 1               | 2               | 0               | 0               | 3     | 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

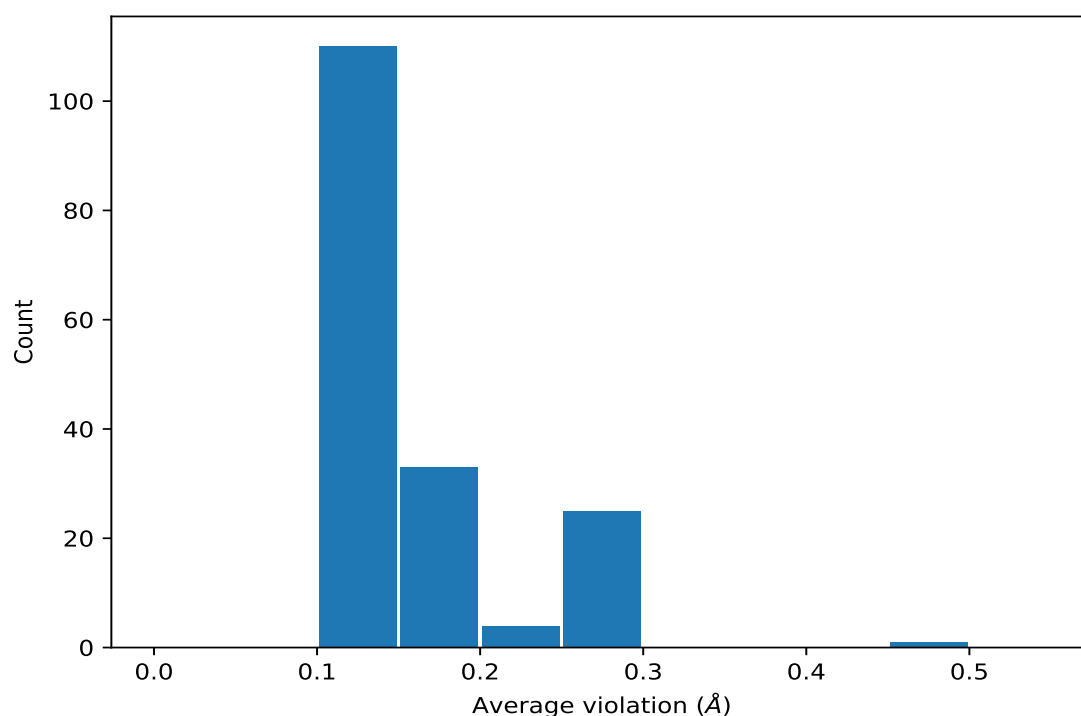
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,3)    | 1:210:A:HIS:NE2  | 2:302:A:ZN:ZN    | 20                  | 0.22     | 0.01                | 0.22       |
| (3,5)    | 2:301:A:ZN:ZN    | 2:302:A:ZN:ZN    | 20                  | 0.21     | 0.01                | 0.21       |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 20                  | 0.15     | 0.02                | 0.15       |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 20                  | 0.15     | 0.02                | 0.15       |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 20                  | 0.15     | 0.02                | 0.15       |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 20                  | 0.15     | 0.02                | 0.15       |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 20                  | 0.15     | 0.02                | 0.15       |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 20                  | 0.15     | 0.02                | 0.15       |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 20                  | 0.15     | 0.02                | 0.15       |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 20                  | 0.15     | 0.02                | 0.15       |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 20                  | 0.15     | 0.02                | 0.15       |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 20                  | 0.14     | 0.01                | 0.14       |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 20                  | 0.14     | 0.01                | 0.14       |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 20                  | 0.14     | 0.01                | 0.14       |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H    | 20                  | 0.14     | 0.02                | 0.13       |
| (3,4)    | 1:90:A:ASP:OD2   | 2:302:A:ZN:ZN    | 19                  | 0.21     | 0.01                | 0.2        |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2775) | 1:9:A:ILE:HB    | 1:19:A:SER:H     | 19                  | 0.15     | 0.01                | 0.16       |
| (1,2842) | 1:20:A:GLN:HA   | 1:25:A:VAL:H     | 19                  | 0.14     | 0.02                | 0.14       |
| (1,3163) | 1:54:A:LEU:HA   | 1:56:A:ASP:H     | 18                  | 0.15     | 0.02                | 0.15       |
| (1,3413) | 1:68:A:ILE:HD11 | 1:79:A:VAL:H     | 18                  | 0.14     | 0.02                | 0.14       |
| (1,3413) | 1:68:A:ILE:HD12 | 1:79:A:VAL:H     | 18                  | 0.14     | 0.02                | 0.14       |
| (1,3413) | 1:68:A:ILE:HD13 | 1:79:A:VAL:H     | 18                  | 0.14     | 0.02                | 0.14       |
| (1,4092) | 1:87:A:ALA:H    | 1:153:A:ASN:H    | 14                  | 0.14     | 0.02                | 0.13       |
| (1,2685) | 1:54:A:LEU:H    | 1:82:A:VAL:HB    | 14                  | 0.13     | 0.02                | 0.13       |
| (1,4675) | 1:208:A:PRO:HD3 | 1:210:A:HIS:H    | 13                  | 0.14     | 0.03                | 0.13       |
| (1,4699) | 1:213:A:VAL:H   | 1:213:A:VAL:HB   | 13                  | 0.12     | 0.01                | 0.12       |
| (1,2790) | 1:7:A:THR:HA    | 1:20:A:GLN:H     | 11                  | 0.14     | 0.01                | 0.13       |
| (1,2097) | 1:58:A:SER:HB2  | 1:67:A:LEU:HG    | 10                  | 0.12     | 0.01                | 0.11       |
| (1,4040) | 1:148:A:GLY:H   | 1:151:A:GLU:H    | 10                  | 0.11     | 0.01                | 0.11       |
| (1,3058) | 1:46:A:LEU:H    | 1:54:A:LEU:HB3   | 9                   | 0.14     | 0.03                | 0.14       |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG11   | 8                   | 0.15     | 0.0                 | 0.15       |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG12   | 8                   | 0.15     | 0.0                 | 0.15       |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG13   | 8                   | 0.15     | 0.0                 | 0.15       |
| (1,3799) | 1:113:A:GLU:HB2 | 1:116:A:LYS:H    | 8                   | 0.15     | 0.04                | 0.14       |
| (1,3799) | 1:113:A:GLU:HB3 | 1:116:A:LYS:H    | 8                   | 0.15     | 0.04                | 0.14       |
| (1,2800) | 1:8:A:VAL:HB    | 1:20:A:GLN:H     | 8                   | 0.14     | 0.01                | 0.14       |
| (1,2518) | 1:195:A:ASN:HB3 | 1:198:A:LYS:HB2  | 8                   | 0.13     | 0.01                | 0.12       |
| (1,2518) | 1:195:A:ASN:HB3 | 1:198:A:LYS:HB3  | 8                   | 0.13     | 0.01                | 0.12       |
| (1,6653) | 1:214:A:GLY:HA3 | 1:215:A:ASP:HB2  | 7                   | 0.19     | 0.01                | 0.19       |
| (1,6653) | 1:214:A:GLY:HA3 | 1:215:A:ASP:HB3  | 7                   | 0.19     | 0.01                | 0.19       |
| (3,2)    | 1:168:A:CYS:SG  | 2:302:A:ZN:ZN    | 7                   | 0.18     | 0.04                | 0.2        |
| (1,6659) | 1:215:A:ASP:HB2 | 1:216:A:LYS:HA   | 7                   | 0.17     | 0.0                 | 0.17       |
| (1,6659) | 1:215:A:ASP:HB3 | 1:216:A:LYS:HA   | 7                   | 0.17     | 0.0                 | 0.17       |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD21 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD22 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD23 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,5457) | 1:39:A:VAL:HG11 | 1:59:A:TRP:HE1   | 6                   | 0.13     | 0.01                | 0.12       |
| (1,5457) | 1:39:A:VAL:HG12 | 1:59:A:TRP:HE1   | 6                   | 0.13     | 0.01                | 0.12       |
| (1,5457) | 1:39:A:VAL:HG13 | 1:59:A:TRP:HE1   | 6                   | 0.13     | 0.01                | 0.12       |
| (1,5457) | 1:39:A:VAL:HG21 | 1:59:A:TRP:HE1   | 6                   | 0.13     | 0.01                | 0.12       |
| (1,5457) | 1:39:A:VAL:HG22 | 1:59:A:TRP:HE1   | 6                   | 0.13     | 0.01                | 0.12       |
| (1,5457) | 1:39:A:VAL:HG23 | 1:59:A:TRP:HE1   | 6                   | 0.13     | 0.01                | 0.12       |
| (1,795)  | 1:57:A:SER:H    | 1:92:A:ILE:HG21  | 5                   | 0.16     | 0.01                | 0.17       |
| (1,795)  | 1:57:A:SER:H    | 1:92:A:ILE:HG22  | 5                   | 0.16     | 0.01                | 0.17       |
| (1,795)  | 1:57:A:SER:H    | 1:92:A:ILE:HG23  | 5                   | 0.16     | 0.01                | 0.17       |
| (1,4940) | 1:115:A:ALA:H   | 1:120:A:TYR:HD1  | 5                   | 0.14     | 0.01                | 0.14       |
| (1,4940) | 1:115:A:ALA:H   | 1:120:A:TYR:HD2  | 5                   | 0.14     | 0.01                | 0.14       |
| (1,3572) | 1:95:A:ILE:H    | 1:120:A:TYR:HE1  | 5                   | 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) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3572) | 1:95:A:ILE:H     | 1:120:A:TYR:HE2 | 5                   | 0.14     | 0.02                | 0.14       |
| (3,1)    | 1:149:A:HIS:NE2  | 2:301:A:ZN:ZN   | 5                   | 0.14     | 0.03                | 0.13       |
| (1,3701) | 1:83:A:ILE:HA    | 1:107:A:SER:H   | 5                   | 0.13     | 0.03                | 0.12       |
| (1,773)  | 1:84:A:ILE:HD11  | 1:92:A:ILE:HB   | 5                   | 0.13     | 0.01                | 0.13       |
| (1,773)  | 1:84:A:ILE:HD12  | 1:92:A:ILE:HB   | 5                   | 0.13     | 0.01                | 0.13       |
| (1,773)  | 1:84:A:ILE:HD13  | 1:92:A:ILE:HB   | 5                   | 0.13     | 0.01                | 0.13       |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB1 | 5                   | 0.12     | 0.01                | 0.12       |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB2 | 5                   | 0.12     | 0.01                | 0.12       |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB3 | 5                   | 0.12     | 0.01                | 0.12       |
| (1,2618) | 1:57:A:SER:HA    | 1:91:A:ARG:HA   | 5                   | 0.12     | 0.01                | 0.12       |
| (1,5671) | 1:54:A:LEU:HD11  | 1:55:A:VAL:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,5671) | 1:54:A:LEU:HD12  | 1:55:A:VAL:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,5671) | 1:54:A:LEU:HD13  | 1:55:A:VAL:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,5671) | 1:54:A:LEU:HD21  | 1:55:A:VAL:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,5671) | 1:54:A:LEU:HD22  | 1:55:A:VAL:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,5671) | 1:54:A:LEU:HD23  | 1:55:A:VAL:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,1406) | 1:84:A:ILE:HG21  | 1:91:A:ARG:HA   | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1406) | 1:84:A:ILE:HG22  | 1:91:A:ARG:HA   | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1406) | 1:84:A:ILE:HG23  | 1:91:A:ARG:HA   | 5                   | 0.11     | 0.01                | 0.11       |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD11 | 5                   | 0.11     | 0.01                | 0.1        |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD12 | 5                   | 0.11     | 0.01                | 0.1        |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD13 | 5                   | 0.11     | 0.01                | 0.1        |
| (1,2053) | 1:45:A:VAL:HA    | 1:53:A:VAL:HG21 | 4                   | 0.17     | 0.04                | 0.18       |
| (1,2053) | 1:45:A:VAL:HA    | 1:53:A:VAL:HG22 | 4                   | 0.17     | 0.04                | 0.18       |
| (1,2053) | 1:45:A:VAL:HA    | 1:53:A:VAL:HG23 | 4                   | 0.17     | 0.04                | 0.18       |
| (1,370)  | 1:28:A:HIS:H     | 1:42:A:ASN:HA   | 4                   | 0.13     | 0.02                | 0.13       |
| (1,2130) | 1:219:A:LEU:HD11 | 1:222:A:THR:HG1 | 4                   | 0.13     | 0.02                | 0.13       |
| (1,2130) | 1:219:A:LEU:HD12 | 1:222:A:THR:HG1 | 4                   | 0.13     | 0.02                | 0.13       |
| (1,2130) | 1:219:A:LEU:HD13 | 1:222:A:THR:HG1 | 4                   | 0.13     | 0.02                | 0.13       |
| (1,2166) | 1:83:A:ILE:HG21  | 1:107:A:SER:H   | 4                   | 0.12     | 0.02                | 0.11       |
| (1,2166) | 1:83:A:ILE:HG22  | 1:107:A:SER:H   | 4                   | 0.12     | 0.02                | 0.11       |
| (1,2166) | 1:83:A:ILE:HG23  | 1:107:A:SER:H   | 4                   | 0.12     | 0.02                | 0.11       |
| (1,3173) | 1:58:A:SER:H     | 1:95:A:ILE:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (1,5878) | 1:90:A:ASP:HB2   | 1:91:A:ARG:HB2  | 3                   | 0.17     | 0.01                | 0.17       |
| (1,5878) | 1:90:A:ASP:HB2   | 1:91:A:ARG:HB3  | 3                   | 0.17     | 0.01                | 0.17       |
| (1,5878) | 1:90:A:ASP:HB3   | 1:91:A:ARG:HB2  | 3                   | 0.17     | 0.01                | 0.17       |
| (1,5878) | 1:90:A:ASP:HB3   | 1:91:A:ARG:HB3  | 3                   | 0.17     | 0.01                | 0.17       |
| (1,1447) | 1:190:A:SER:HB2  | 1:226:A:LEU:HB2 | 3                   | 0.16     | 0.0                 | 0.16       |
| (1,1447) | 1:190:A:SER:HB2  | 1:226:A:LEU:HB3 | 3                   | 0.16     | 0.0                 | 0.16       |
| (1,1447) | 1:190:A:SER:HB3  | 1:226:A:LEU:HB2 | 3                   | 0.16     | 0.0                 | 0.16       |
| (1,1447) | 1:190:A:SER:HB3  | 1:226:A:LEU:HB3 | 3                   | 0.16     | 0.0                 | 0.16       |
| (1,4800) | 1:224:A:ASP:H    | 1:226:A:LEU:HB2 | 3                   | 0.16     | 0.0                 | 0.16       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,4800) | 1:224:A:ASP:H    | 1:226:A:LEU:HB3  | 3                   | 0.16     | 0.0                 | 0.16       |
| (1,2963) | 1:32:A:GLY:HA2   | 1:33:A:SER:H     | 3                   | 0.14     | 0.02                | 0.13       |
| (1,3168) | 1:56:A:ASP:H     | 1:57:A:SER:H     | 3                   | 0.13     | 0.03                | 0.11       |
| (1,317)  | 1:186:A:VAL:HG21 | 1:187:A:ASN:HB2  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,317)  | 1:186:A:VAL:HG21 | 1:187:A:ASN:HB3  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,317)  | 1:186:A:VAL:HG22 | 1:187:A:ASN:HB2  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,317)  | 1:186:A:VAL:HG22 | 1:187:A:ASN:HB3  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,317)  | 1:186:A:VAL:HG23 | 1:187:A:ASN:HB2  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,317)  | 1:186:A:VAL:HG23 | 1:187:A:ASN:HB3  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,899)  | 1:109:A:ALA:HB1  | 1:113:A:GLU:H    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,899)  | 1:109:A:ALA:HB2  | 1:113:A:GLU:H    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,899)  | 1:109:A:ALA:HB3  | 1:113:A:GLU:H    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,4796) | 1:222:A:THR:HG1  | 1:224:A:ASP:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,3433) | 1:81:A:ASP:H     | 1:82:A:VAL:HB    | 2                   | 0.46     | 0.0                 | 0.46       |
| (1,5795) | 1:71:A:VAL:HG21  | 1:79:A:VAL:HG11  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG21  | 1:79:A:VAL:HG12  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG21  | 1:79:A:VAL:HG13  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG21  | 1:79:A:VAL:HG21  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG21  | 1:79:A:VAL:HG22  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG21  | 1:79:A:VAL:HG23  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG22  | 1:79:A:VAL:HG11  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG22  | 1:79:A:VAL:HG12  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG22  | 1:79:A:VAL:HG13  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG22  | 1:79:A:VAL:HG21  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG22  | 1:79:A:VAL:HG22  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG22  | 1:79:A:VAL:HG23  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG23  | 1:79:A:VAL:HG11  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG23  | 1:79:A:VAL:HG12  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG23  | 1:79:A:VAL:HG13  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG23  | 1:79:A:VAL:HG21  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG23  | 1:79:A:VAL:HG22  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,5795) | 1:71:A:VAL:HG23  | 1:79:A:VAL:HG23  | 2                   | 0.28     | 0.03                | 0.28       |
| (1,2104) | 1:68:A:ILE:HB    | 1:79:A:VAL:HB    | 2                   | 0.27     | 0.07                | 0.27       |
| (1,5679) | 1:55:A:VAL:HA    | 1:82:A:VAL:HG11  | 2                   | 0.26     | 0.03                | 0.26       |
| (1,5679) | 1:55:A:VAL:HA    | 1:82:A:VAL:HG12  | 2                   | 0.26     | 0.03                | 0.26       |
| (1,5679) | 1:55:A:VAL:HA    | 1:82:A:VAL:HG13  | 2                   | 0.26     | 0.03                | 0.26       |
| (1,5679) | 1:55:A:VAL:HA    | 1:82:A:VAL:HG21  | 2                   | 0.26     | 0.03                | 0.26       |
| (1,5679) | 1:55:A:VAL:HA    | 1:82:A:VAL:HG22  | 2                   | 0.26     | 0.03                | 0.26       |
| (1,5679) | 1:55:A:VAL:HA    | 1:82:A:VAL:HG23  | 2                   | 0.26     | 0.03                | 0.26       |
| (1,1154) | 1:172:A:SER:HA   | 1:173:A:THR:HB   | 2                   | 0.22     | 0.03                | 0.22       |
| (1,2836) | 1:173:A:THR:H    | 1:173:A:THR:HG21 | 2                   | 0.16     | 0.01                | 0.16       |
| (1,2836) | 1:173:A:THR:H    | 1:173:A:THR:HG22 | 2                   | 0.16     | 0.01                | 0.16       |

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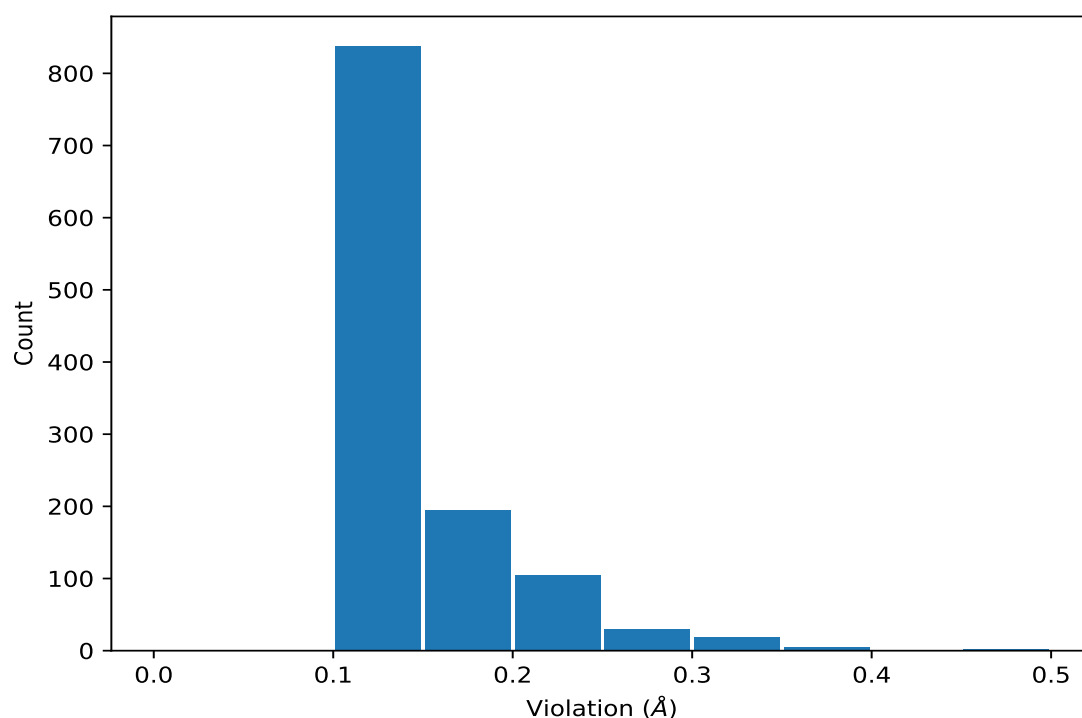
| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2836) | 1:173:A:THR:H   | 1:173:A:THR:HG23 | 2                   | 0.16     | 0.01                | 0.16       |
| (1,686)  | 1:81:A:ASP:HA   | 1:82:A:VAL:HB    | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,5411) | 1:32:A:GLY:HA2  | 1:33:A:SER:H     | 2                   | 0.16     | 0.06                | 0.16       |
| (1,5411) | 1:32:A:GLY:HA3  | 1:33:A:SER:H     | 2                   | 0.16     | 0.06                | 0.16       |
| (1,5440) | 1:35:A:ASN:HD21 | 1:39:A:VAL:HG11  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,5440) | 1:35:A:ASN:HD21 | 1:39:A:VAL:HG12  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,5440) | 1:35:A:ASN:HD21 | 1:39:A:VAL:HG13  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,5440) | 1:35:A:ASN:HD21 | 1:39:A:VAL:HG21  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,5440) | 1:35:A:ASN:HD21 | 1:39:A:VAL:HG22  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,5440) | 1:35:A:ASN:HD21 | 1:39:A:VAL:HG23  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,2394) | 1:114:A:LEU:HB2 | 1:150:A:THR:HB   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,3170) | 1:57:A:SER:H    | 1:84:A:ILE:HA    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,3196) | 1:30:A:GLU:HA   | 1:59:A:TRP:HE1   | 2                   | 0.12     | 0.02                | 0.12       |
| (2,9)    | 1:67:A:LEU:HD21 | 1:71:A:VAL:H     | 2                   | 0.12     | 0.02                | 0.12       |
| (2,9)    | 1:67:A:LEU:HD22 | 1:71:A:VAL:H     | 2                   | 0.12     | 0.02                | 0.12       |
| (2,9)    | 1:67:A:LEU:HD23 | 1:71:A:VAL:H     | 2                   | 0.12     | 0.02                | 0.12       |
| (1,39)   | 1:34:A:PHE:HD1  | 1:39:A:VAL:HB    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,39)   | 1:34:A:PHE:HD2  | 1:39:A:VAL:HB    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1463) | 1:190:A:SER:HA  | 1:226:A:LEU:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1463) | 1:190:A:SER:HA  | 1:226:A:LEU:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2875) | 1:22:A:ASN:H    | 1:26:A:TRP:HE1   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,3100) | 1:48:A:THR:H    | 1:51:A:GLY:HA2   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,6722) | 1:227:A:LYS:H   | 1:227:A:LYS:HG2  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,6722) | 1:227:A:LYS:H   | 1:227:A:LYS:HG3  | 2                   | 0.11     | 0.01                | 0.11       |
| (2,6)    | 1:32:A:GLY:H    | 1:40:A:PRO:HB2   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,6691) | 1:222:A:THR:HA  | 1:223:A:LEU:HD11 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,6691) | 1:222:A:THR:HA  | 1:223:A:LEU:HD12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,6691) | 1:222:A:THR:HA  | 1:223:A:LEU:HD13 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,6691) | 1:222:A:THR:HA  | 1:223:A:LEU:HD21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,6691) | 1:222:A:THR:HA  | 1:223:A:LEU:HD22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,6691) | 1:222:A:THR:HA  | 1:223:A:LEU:HD23 | 2                   | 0.11     | 0.0                 | 0.11       |

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

## 9.5 All violated distance restraints [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) |
|----------|------------------|-----------------|----------|---------------|
| (1,3433) | 1:81:A:ASP:H     | 1:82:A:VAL:HB   | 20       | 0.47          |
| (1,3433) | 1:81:A:ASP:H     | 1:82:A:VAL:HB   | 13       | 0.46          |
| (1,5895) | 1:95:A:ILE:HG13  | 1:121:A:GLU:HB2 | 18       | 0.38          |
| (1,5895) | 1:95:A:ILE:HG13  | 1:121:A:GLU:HB3 | 18       | 0.38          |
| (1,982)  | 1:150:A:THR:HG21 | 1:152:A:ASP:H   | 10       | 0.36          |
| (1,982)  | 1:150:A:THR:HG22 | 1:152:A:ASP:H   | 10       | 0.36          |
| (1,982)  | 1:150:A:THR:HG23 | 1:152:A:ASP:H   | 10       | 0.36          |
| (1,2104) | 1:68:A:ILE:HB    | 1:79:A:VAL:HB   | 9        | 0.34          |
| (1,5795) | 1:71:A:VAL:HG21  | 1:79:A:VAL:HG11 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG21  | 1:79:A:VAL:HG12 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG21  | 1:79:A:VAL:HG13 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG21  | 1:79:A:VAL:HG21 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG21  | 1:79:A:VAL:HG22 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG21  | 1:79:A:VAL:HG23 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG22  | 1:79:A:VAL:HG11 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG22  | 1:79:A:VAL:HG12 | 9        | 0.31          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,5795) | 1:71:A:VAL:HG22 | 1:79:A:VAL:HG13 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG22 | 1:79:A:VAL:HG21 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG22 | 1:79:A:VAL:HG22 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG22 | 1:79:A:VAL:HG23 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG23 | 1:79:A:VAL:HG11 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG23 | 1:79:A:VAL:HG12 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG23 | 1:79:A:VAL:HG13 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG23 | 1:79:A:VAL:HG21 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG23 | 1:79:A:VAL:HG22 | 9        | 0.31          |
| (1,5795) | 1:71:A:VAL:HG23 | 1:79:A:VAL:HG23 | 9        | 0.31          |
| (1,5679) | 1:55:A:VAL:HA   | 1:82:A:VAL:HG11 | 20       | 0.29          |
| (1,5679) | 1:55:A:VAL:HA   | 1:82:A:VAL:HG12 | 20       | 0.29          |
| (1,5679) | 1:55:A:VAL:HA   | 1:82:A:VAL:HG13 | 20       | 0.29          |
| (1,5679) | 1:55:A:VAL:HA   | 1:82:A:VAL:HG21 | 20       | 0.29          |
| (1,5679) | 1:55:A:VAL:HA   | 1:82:A:VAL:HG22 | 20       | 0.29          |
| (1,5679) | 1:55:A:VAL:HA   | 1:82:A:VAL:HG23 | 20       | 0.29          |
| (1,4075) | 1:150:A:THR:HA  | 1:151:A:GLU:H   | 10       | 0.28          |
| (1,770)  | 1:96:A:LYS:HA   | 1:121:A:GLU:HG3 | 18       | 0.27          |
| (1,3206) | 1:39:A:VAL:HB   | 1:59:A:TRP:HE1  | 12       | 0.26          |
| (1,5795) | 1:71:A:VAL:HG21 | 1:79:A:VAL:HG11 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG21 | 1:79:A:VAL:HG12 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG21 | 1:79:A:VAL:HG13 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG21 | 1:79:A:VAL:HG21 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG21 | 1:79:A:VAL:HG22 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG21 | 1:79:A:VAL:HG23 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG22 | 1:79:A:VAL:HG11 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG22 | 1:79:A:VAL:HG12 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG22 | 1:79:A:VAL:HG13 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG22 | 1:79:A:VAL:HG21 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG22 | 1:79:A:VAL:HG22 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG22 | 1:79:A:VAL:HG23 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG23 | 1:79:A:VAL:HG11 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG23 | 1:79:A:VAL:HG12 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG23 | 1:79:A:VAL:HG13 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG23 | 1:79:A:VAL:HG21 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG23 | 1:79:A:VAL:HG22 | 14       | 0.25          |
| (1,5795) | 1:71:A:VAL:HG23 | 1:79:A:VAL:HG23 | 14       | 0.25          |
| (1,5439) | 1:35:A:ASN:HB2  | 1:37:A:GLU:H    | 19       | 0.25          |
| (1,5439) | 1:35:A:ASN:HB3  | 1:37:A:GLU:H    | 19       | 0.25          |
| (1,1154) | 1:172:A:SER:HA  | 1:173:A:THR:HB  | 6        | 0.25          |
| (1,1901) | 1:8:A:VAL:HG21  | 1:19:A:SER:HA   | 10       | 0.24          |
| (1,1901) | 1:8:A:VAL:HG22  | 1:19:A:SER:HA   | 10       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1901) | 1:8:A:VAL:HG23  | 1:19:A:SER:HA   | 10       | 0.24          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 9        | 0.23          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 15       | 0.23          |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 6        | 0.23          |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 7        | 0.23          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 5        | 0.23          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 6        | 0.23          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 7        | 0.23          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 15       | 0.23          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 2        | 0.22          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 5        | 0.22          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 8        | 0.22          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 17       | 0.22          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 18       | 0.22          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 19       | 0.22          |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 12       | 0.22          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 1        | 0.22          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 2        | 0.22          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 8        | 0.22          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 9        | 0.22          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 12       | 0.22          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 17       | 0.22          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 18       | 0.22          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 19       | 0.22          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 20       | 0.22          |
| (1,5679) | 1:55:A:VAL:HA   | 1:82:A:VAL:HG11 | 13       | 0.22          |
| (1,5679) | 1:55:A:VAL:HA   | 1:82:A:VAL:HG12 | 13       | 0.22          |
| (1,5679) | 1:55:A:VAL:HA   | 1:82:A:VAL:HG13 | 13       | 0.22          |
| (1,5679) | 1:55:A:VAL:HA   | 1:82:A:VAL:HG21 | 13       | 0.22          |
| (1,5679) | 1:55:A:VAL:HA   | 1:82:A:VAL:HG22 | 13       | 0.22          |
| (1,5679) | 1:55:A:VAL:HA   | 1:82:A:VAL:HG23 | 13       | 0.22          |
| (1,5411) | 1:32:A:GLY:HA2  | 1:33:A:SER:H    | 19       | 0.22          |
| (1,5411) | 1:32:A:GLY:HA3  | 1:33:A:SER:H    | 19       | 0.22          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 1        | 0.21          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 4        | 0.21          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 6        | 0.21          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 7        | 0.21          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 11       | 0.21          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 12       | 0.21          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 14       | 0.21          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 20       | 0.21          |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 2        | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 3        | 0.21          |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 5        | 0.21          |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 11       | 0.21          |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 19       | 0.21          |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 20       | 0.21          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 3        | 0.21          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 4        | 0.21          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 11       | 0.21          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 14       | 0.21          |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 16       | 0.21          |
| (3,2)    | 1:168:A:CYS:SG  | 2:302:A:ZN:ZN   | 6        | 0.21          |
| (3,2)    | 1:168:A:CYS:SG  | 2:302:A:ZN:ZN   | 7        | 0.21          |
| (1,6653) | 1:214:A:GLY:HA3 | 1:215:A:ASP:HB2 | 4        | 0.21          |
| (1,6653) | 1:214:A:GLY:HA3 | 1:215:A:ASP:HB3 | 4        | 0.21          |
| (1,3163) | 1:54:A:LEU:HA   | 1:56:A:ASP:H    | 13       | 0.21          |
| (1,2053) | 1:45:A:VAL:HA   | 1:53:A:VAL:HG21 | 6        | 0.21          |
| (1,2053) | 1:45:A:VAL:HA   | 1:53:A:VAL:HG22 | 6        | 0.21          |
| (1,2053) | 1:45:A:VAL:HA   | 1:53:A:VAL:HG23 | 6        | 0.21          |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 3        | 0.2           |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 13       | 0.2           |
| (3,5)    | 2:301:A:ZN:ZN   | 2:302:A:ZN:ZN   | 16       | 0.2           |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 1        | 0.2           |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 4        | 0.2           |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 9        | 0.2           |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 10       | 0.2           |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 13       | 0.2           |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 14       | 0.2           |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 15       | 0.2           |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 16       | 0.2           |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 17       | 0.2           |
| (3,4)    | 1:90:A:ASP:OD2  | 2:302:A:ZN:ZN   | 18       | 0.2           |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 10       | 0.2           |
| (3,3)    | 1:210:A:HIS:NE2 | 2:302:A:ZN:ZN   | 13       | 0.2           |
| (3,2)    | 1:168:A:CYS:SG  | 2:302:A:ZN:ZN   | 3        | 0.2           |
| (3,2)    | 1:168:A:CYS:SG  | 2:302:A:ZN:ZN   | 10       | 0.2           |
| (3,1)    | 1:149:A:HIS:NE2 | 2:301:A:ZN:ZN   | 11       | 0.2           |
| (1,6653) | 1:214:A:GLY:HA3 | 1:215:A:ASP:HB2 | 12       | 0.2           |
| (1,6653) | 1:214:A:GLY:HA3 | 1:215:A:ASP:HB3 | 12       | 0.2           |
| (1,6653) | 1:214:A:GLY:HA3 | 1:215:A:ASP:HB2 | 18       | 0.2           |
| (1,6653) | 1:214:A:GLY:HA3 | 1:215:A:ASP:HB3 | 18       | 0.2           |
| (1,5440) | 1:35:A:ASN:HD21 | 1:39:A:VAL:HG11 | 14       | 0.2           |
| (1,5440) | 1:35:A:ASN:HD21 | 1:39:A:VAL:HG12 | 14       | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,5440) | 1:35:A:ASN:HD21  | 1:39:A:VAL:HG13  | 14       | 0.2           |
| (1,5440) | 1:35:A:ASN:HD21  | 1:39:A:VAL:HG21  | 14       | 0.2           |
| (1,5440) | 1:35:A:ASN:HD21  | 1:39:A:VAL:HG22  | 14       | 0.2           |
| (1,5440) | 1:35:A:ASN:HD21  | 1:39:A:VAL:HG23  | 14       | 0.2           |
| (1,4675) | 1:208:A:PRO:HD3  | 1:210:A:HIS:H    | 12       | 0.2           |
| (1,3867) | 1:95:A:ILE:HG13  | 1:121:A:GLU:H    | 18       | 0.2           |
| (1,3799) | 1:113:A:GLU:HB2  | 1:116:A:LYS:H    | 8        | 0.2           |
| (1,3799) | 1:113:A:GLU:HB3  | 1:116:A:LYS:H    | 8        | 0.2           |
| (1,3058) | 1:46:A:LEU:H     | 1:54:A:LEU:HB3   | 18       | 0.2           |
| (1,2104) | 1:68:A:ILE:HB    | 1:79:A:VAL:HB    | 14       | 0.2           |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 19       | 0.2           |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 19       | 0.2           |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 19       | 0.2           |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 19       | 0.2           |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 19       | 0.2           |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 19       | 0.2           |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 19       | 0.2           |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 19       | 0.2           |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 19       | 0.2           |
| (1,6653) | 1:214:A:GLY:HA3  | 1:215:A:ASP:HB2  | 6        | 0.19          |
| (1,6653) | 1:214:A:GLY:HA3  | 1:215:A:ASP:HB3  | 6        | 0.19          |
| (1,5809) | 1:78:A:ARG:HA    | 1:79:A:VAL:HG11  | 14       | 0.19          |
| (1,5809) | 1:78:A:ARG:HA    | 1:79:A:VAL:HG12  | 14       | 0.19          |
| (1,5809) | 1:78:A:ARG:HA    | 1:79:A:VAL:HG13  | 14       | 0.19          |
| (1,5809) | 1:78:A:ARG:HA    | 1:79:A:VAL:HG21  | 14       | 0.19          |
| (1,5809) | 1:78:A:ARG:HA    | 1:79:A:VAL:HG22  | 14       | 0.19          |
| (1,5809) | 1:78:A:ARG:HA    | 1:79:A:VAL:HG23  | 14       | 0.19          |
| (1,4675) | 1:208:A:PRO:HD3  | 1:210:A:HIS:H    | 10       | 0.19          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H    | 11       | 0.19          |
| (1,3799) | 1:113:A:GLU:HB2  | 1:116:A:LYS:H    | 18       | 0.19          |
| (1,3799) | 1:113:A:GLU:HB3  | 1:116:A:LYS:H    | 18       | 0.19          |
| (1,3701) | 1:83:A:ILE:HA    | 1:107:A:SER:H    | 15       | 0.19          |
| (1,1161) | 1:171:A:LYS:H    | 1:175:A:ALA:HB1  | 11       | 0.19          |
| (1,1161) | 1:171:A:LYS:H    | 1:175:A:ALA:HB2  | 11       | 0.19          |
| (1,1161) | 1:171:A:LYS:H    | 1:175:A:ALA:HB3  | 11       | 0.19          |
| (1,1154) | 1:172:A:SER:HA   | 1:173:A:THR:HB   | 11       | 0.19          |
| (3,2)    | 1:168:A:CYS:SG   | 2:302:A:ZN:ZN    | 16       | 0.18          |
| (1,6653) | 1:214:A:GLY:HA3  | 1:215:A:ASP:HB2  | 2        | 0.18          |
| (1,6653) | 1:214:A:GLY:HA3  | 1:215:A:ASP:HB3  | 2        | 0.18          |
| (1,6653) | 1:214:A:GLY:HA3  | 1:215:A:ASP:HB2  | 13       | 0.18          |
| (1,6653) | 1:214:A:GLY:HA3  | 1:215:A:ASP:HB3  | 13       | 0.18          |
| (1,5878) | 1:90:A:ASP:HB2   | 1:91:A:ARG:HB2   | 6        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,5878) | 1:90:A:ASP:HB2   | 1:91:A:ARG:HB3   | 6        | 0.18          |
| (1,5878) | 1:90:A:ASP:HB3   | 1:91:A:ARG:HB2   | 6        | 0.18          |
| (1,5878) | 1:90:A:ASP:HB3   | 1:91:A:ARG:HB3   | 6        | 0.18          |
| (1,4092) | 1:87:A:ALA:H     | 1:153:A:ASN:H    | 13       | 0.18          |
| (1,3799) | 1:113:A:GLU:HB2  | 1:116:A:LYS:H    | 3        | 0.18          |
| (1,3799) | 1:113:A:GLU:HB3  | 1:116:A:LYS:H    | 3        | 0.18          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H     | 14       | 0.18          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H     | 14       | 0.18          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H     | 14       | 0.18          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H     | 16       | 0.18          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H     | 16       | 0.18          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H     | 16       | 0.18          |
| (1,3168) | 1:56:A:ASP:H     | 1:57:A:SER:H     | 20       | 0.18          |
| (1,3058) | 1:46:A:LEU:H     | 1:54:A:LEU:HB3   | 5        | 0.18          |
| (1,2757) | 1:8:A:VAL:HA     | 1:18:A:ILE:H     | 10       | 0.18          |
| (1,2053) | 1:45:A:VAL:HA    | 1:53:A:VAL:HG21  | 5        | 0.18          |
| (1,2053) | 1:45:A:VAL:HA    | 1:53:A:VAL:HG22  | 5        | 0.18          |
| (1,2053) | 1:45:A:VAL:HA    | 1:53:A:VAL:HG23  | 5        | 0.18          |
| (1,2053) | 1:45:A:VAL:HA    | 1:53:A:VAL:HG21  | 18       | 0.18          |
| (1,2053) | 1:45:A:VAL:HA    | 1:53:A:VAL:HG22  | 18       | 0.18          |
| (1,2053) | 1:45:A:VAL:HA    | 1:53:A:VAL:HG23  | 18       | 0.18          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG21  | 16       | 0.18          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG22  | 16       | 0.18          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG23  | 16       | 0.18          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 20       | 0.18          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 20       | 0.18          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 20       | 0.18          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 20       | 0.18          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 20       | 0.18          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 20       | 0.18          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 20       | 0.18          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 20       | 0.18          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 20       | 0.18          |
| (3,5)    | 2:301:A:ZN:ZN    | 2:302:A:ZN:ZN    | 10       | 0.17          |
| (1,6659) | 1:215:A:ASP:HB2  | 1:216:A:LYS:HA   | 2        | 0.17          |
| (1,6659) | 1:215:A:ASP:HB3  | 1:216:A:LYS:HA   | 2        | 0.17          |
| (1,6659) | 1:215:A:ASP:HB2  | 1:216:A:LYS:HA   | 4        | 0.17          |
| (1,6659) | 1:215:A:ASP:HB3  | 1:216:A:LYS:HA   | 4        | 0.17          |
| (1,6659) | 1:215:A:ASP:HB2  | 1:216:A:LYS:HA   | 12       | 0.17          |
| (1,6659) | 1:215:A:ASP:HB3  | 1:216:A:LYS:HA   | 12       | 0.17          |
| (1,6659) | 1:215:A:ASP:HB2  | 1:216:A:LYS:HA   | 18       | 0.17          |
| (1,6659) | 1:215:A:ASP:HB3  | 1:216:A:LYS:HA   | 18       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,6653) | 1:214:A:GLY:HA3  | 1:215:A:ASP:HB2  | 10       | 0.17          |
| (1,6653) | 1:214:A:GLY:HA3  | 1:215:A:ASP:HB3  | 10       | 0.17          |
| (1,5878) | 1:90:A:ASP:HB2   | 1:91:A:ARG:HB2   | 5        | 0.17          |
| (1,5878) | 1:90:A:ASP:HB2   | 1:91:A:ARG:HB3   | 5        | 0.17          |
| (1,5878) | 1:90:A:ASP:HB3   | 1:91:A:ARG:HB2   | 5        | 0.17          |
| (1,5878) | 1:90:A:ASP:HB3   | 1:91:A:ARG:HB3   | 5        | 0.17          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H    | 15       | 0.17          |
| (1,4092) | 1:87:A:ALA:H     | 1:153:A:ASN:H    | 5        | 0.17          |
| (1,3572) | 1:95:A:ILE:H     | 1:120:A:TYR:HE1  | 16       | 0.17          |
| (1,3572) | 1:95:A:ILE:H     | 1:120:A:TYR:HE2  | 16       | 0.17          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H     | 1        | 0.17          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H     | 4        | 0.17          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H     | 17       | 0.17          |
| (1,2836) | 1:173:A:THR:H    | 1:173:A:THR:HG21 | 6        | 0.17          |
| (1,2836) | 1:173:A:THR:H    | 1:173:A:THR:HG22 | 6        | 0.17          |
| (1,2836) | 1:173:A:THR:H    | 1:173:A:THR:HG23 | 6        | 0.17          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H     | 8        | 0.17          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H     | 20       | 0.17          |
| (1,2685) | 1:54:A:LEU:H     | 1:82:A:VAL:HB    | 18       | 0.17          |
| (1,1986) | 1:34:A:PHE:HB2   | 1:39:A:VAL:HG11  | 20       | 0.17          |
| (1,1986) | 1:34:A:PHE:HB2   | 1:39:A:VAL:HG12  | 20       | 0.17          |
| (1,1986) | 1:34:A:PHE:HB2   | 1:39:A:VAL:HG13  | 20       | 0.17          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG21  | 17       | 0.17          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG22  | 17       | 0.17          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG23  | 17       | 0.17          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG21  | 19       | 0.17          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG22  | 19       | 0.17          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG23  | 19       | 0.17          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 2        | 0.17          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 2        | 0.17          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 2        | 0.17          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 2        | 0.17          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 2        | 0.17          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 2        | 0.17          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 2        | 0.17          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 2        | 0.17          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 2        | 0.17          |
| (1,6659) | 1:215:A:ASP:HB2  | 1:216:A:LYS:HA   | 6        | 0.16          |
| (1,6659) | 1:215:A:ASP:HB3  | 1:216:A:LYS:HA   | 6        | 0.16          |
| (1,6659) | 1:215:A:ASP:HB2  | 1:216:A:LYS:HA   | 10       | 0.16          |
| (1,6659) | 1:215:A:ASP:HB3  | 1:216:A:LYS:HA   | 10       | 0.16          |
| (1,6659) | 1:215:A:ASP:HB2  | 1:216:A:LYS:HA   | 13       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,6659) | 1:215:A:ASP:HB3  | 1:216:A:LYS:HA   | 13       | 0.16          |
| (1,4940) | 1:115:A:ALA:H    | 1:120:A:TYR:HD1  | 16       | 0.16          |
| (1,4940) | 1:115:A:ALA:H    | 1:120:A:TYR:HD2  | 16       | 0.16          |
| (1,4800) | 1:224:A:ASP:H    | 1:226:A:LEU:HB2  | 7        | 0.16          |
| (1,4800) | 1:224:A:ASP:H    | 1:226:A:LEU:HB3  | 7        | 0.16          |
| (1,4800) | 1:224:A:ASP:H    | 1:226:A:LEU:HB2  | 19       | 0.16          |
| (1,4800) | 1:224:A:ASP:H    | 1:226:A:LEU:HB3  | 19       | 0.16          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H    | 9        | 0.16          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H    | 17       | 0.16          |
| (1,4092) | 1:87:A:ALA:H     | 1:153:A:ASN:H    | 6        | 0.16          |
| (1,3799) | 1:113:A:GLU:HB2  | 1:116:A:LYS:H    | 15       | 0.16          |
| (1,3799) | 1:113:A:GLU:HB3  | 1:116:A:LYS:H    | 15       | 0.16          |
| (1,3572) | 1:95:A:ILE:H     | 1:120:A:TYR:HE1  | 15       | 0.16          |
| (1,3572) | 1:95:A:ILE:H     | 1:120:A:TYR:HE2  | 15       | 0.16          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H     | 7        | 0.16          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H     | 12       | 0.16          |
| (1,3058) | 1:46:A:LEU:H     | 1:54:A:LEU:HB3   | 6        | 0.16          |
| (1,2963) | 1:32:A:GLY:HA2   | 1:33:A:SER:H     | 20       | 0.16          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H     | 2        | 0.16          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H     | 8        | 0.16          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H     | 9        | 0.16          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H     | 15       | 0.16          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H     | 17       | 0.16          |
| (1,2836) | 1:173:A:THR:H    | 1:173:A:THR:HG21 | 11       | 0.16          |
| (1,2836) | 1:173:A:THR:H    | 1:173:A:THR:HG22 | 11       | 0.16          |
| (1,2836) | 1:173:A:THR:H    | 1:173:A:THR:HG23 | 11       | 0.16          |
| (1,2790) | 1:7:A:THR:HA     | 1:20:A:GLN:H     | 14       | 0.16          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H     | 2        | 0.16          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H     | 6        | 0.16          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H     | 9        | 0.16          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H     | 11       | 0.16          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H     | 13       | 0.16          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H     | 15       | 0.16          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H     | 17       | 0.16          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H     | 19       | 0.16          |
| (1,1447) | 1:190:A:SER:HB2  | 1:226:A:LEU:HB2  | 9        | 0.16          |
| (1,1447) | 1:190:A:SER:HB2  | 1:226:A:LEU:HB3  | 9        | 0.16          |
| (1,1447) | 1:190:A:SER:HB3  | 1:226:A:LEU:HB2  | 9        | 0.16          |
| (1,1447) | 1:190:A:SER:HB3  | 1:226:A:LEU:HB3  | 9        | 0.16          |
| (1,1447) | 1:190:A:SER:HB2  | 1:226:A:LEU:HB2  | 17       | 0.16          |
| (1,1447) | 1:190:A:SER:HB2  | 1:226:A:LEU:HB3  | 17       | 0.16          |
| (1,1447) | 1:190:A:SER:HB3  | 1:226:A:LEU:HB2  | 17       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1447) | 1:190:A:SER:HB3  | 1:226:A:LEU:HB3  | 17       | 0.16          |
| (1,686)  | 1:81:A:ASP:HA    | 1:82:A:VAL:HB    | 13       | 0.16          |
| (1,686)  | 1:81:A:ASP:HA    | 1:82:A:VAL:HB    | 20       | 0.16          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 4        | 0.16          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 4        | 0.16          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 4        | 0.16          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 4        | 0.16          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 4        | 0.16          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 4        | 0.16          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 4        | 0.16          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 4        | 0.16          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 4        | 0.16          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 5        | 0.16          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 5        | 0.16          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 5        | 0.16          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 5        | 0.16          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 5        | 0.16          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 5        | 0.16          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 5        | 0.16          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 5        | 0.16          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 5        | 0.16          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 6        | 0.16          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 6        | 0.16          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 6        | 0.16          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 6        | 0.16          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 6        | 0.16          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 6        | 0.16          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 6        | 0.16          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 6        | 0.16          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 6        | 0.16          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 11       | 0.16          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 11       | 0.16          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 11       | 0.16          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 11       | 0.16          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 11       | 0.16          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 11       | 0.16          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 11       | 0.16          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 11       | 0.16          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 11       | 0.16          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 17       | 0.16          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 17       | 0.16          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 17       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG21 | 19       | 0.16          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG22 | 19       | 0.16          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG23 | 19       | 0.16          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG11  | 2        | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG12  | 2        | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG13  | 2        | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG11  | 6        | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG12  | 6        | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG13  | 6        | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG11  | 8        | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG12  | 8        | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG13  | 8        | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG11  | 9        | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG12  | 9        | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG13  | 9        | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG11  | 15       | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG12  | 15       | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG13  | 15       | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG11  | 17       | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG12  | 17       | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG13  | 17       | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG11  | 18       | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG12  | 18       | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG13  | 18       | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG11  | 20       | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG12  | 20       | 0.15          |
| (2,4)    | 1:7:A:THR:HA    | 1:8:A:VAL:HG13  | 20       | 0.15          |
| (1,5878) | 1:90:A:ASP:HB2  | 1:91:A:ARG:HB2  | 7        | 0.15          |
| (1,5878) | 1:90:A:ASP:HB2  | 1:91:A:ARG:HB3  | 7        | 0.15          |
| (1,5878) | 1:90:A:ASP:HB3  | 1:91:A:ARG:HB2  | 7        | 0.15          |
| (1,5878) | 1:90:A:ASP:HB3  | 1:91:A:ARG:HB3  | 7        | 0.15          |
| (1,5830) | 1:82:A:VAL:HG11 | 1:83:A:ILE:H    | 20       | 0.15          |
| (1,5830) | 1:82:A:VAL:HG12 | 1:83:A:ILE:H    | 20       | 0.15          |
| (1,5830) | 1:82:A:VAL:HG13 | 1:83:A:ILE:H    | 20       | 0.15          |
| (1,5830) | 1:82:A:VAL:HG21 | 1:83:A:ILE:H    | 20       | 0.15          |
| (1,5830) | 1:82:A:VAL:HG22 | 1:83:A:ILE:H    | 20       | 0.15          |
| (1,5830) | 1:82:A:VAL:HG23 | 1:83:A:ILE:H    | 20       | 0.15          |
| (1,5011) | 1:34:A:PHE:HD1  | 1:37:A:GLU:HB2  | 14       | 0.15          |
| (1,5011) | 1:34:A:PHE:HD2  | 1:37:A:GLU:HB2  | 14       | 0.15          |
| (1,4940) | 1:115:A:ALA:H   | 1:120:A:TYR:HD1 | 17       | 0.15          |
| (1,4940) | 1:115:A:ALA:H   | 1:120:A:TYR:HD2 | 17       | 0.15          |
| (1,4800) | 1:224:A:ASP:H   | 1:226:A:LEU:HB2 | 5        | 0.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,4800) | 1:224:A:ASP:H    | 1:226:A:LEU:HB3 | 5        | 0.15          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H   | 3        | 0.15          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H   | 8        | 0.15          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H   | 12       | 0.15          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H   | 19       | 0.15          |
| (1,4092) | 1:87:A:ALA:H     | 1:153:A:ASN:H   | 16       | 0.15          |
| (1,4040) | 1:148:A:GLY:H    | 1:151:A:GLU:H   | 11       | 0.15          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 8        | 0.15          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 8        | 0.15          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 8        | 0.15          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 9        | 0.15          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 9        | 0.15          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 9        | 0.15          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H    | 3        | 0.15          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H    | 9        | 0.15          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H    | 10       | 0.15          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H    | 14       | 0.15          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H    | 15       | 0.15          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H    | 18       | 0.15          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H    | 19       | 0.15          |
| (1,2982) | 1:34:A:PHE:H     | 1:37:A:GLU:H    | 19       | 0.15          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H    | 14       | 0.15          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H    | 18       | 0.15          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H    | 20       | 0.15          |
| (1,2800) | 1:8:A:VAL:HB     | 1:20:A:GLN:H    | 8        | 0.15          |
| (1,2790) | 1:7:A:THR:HA     | 1:20:A:GLN:H    | 1        | 0.15          |
| (1,2790) | 1:7:A:THR:HA     | 1:20:A:GLN:H    | 3        | 0.15          |
| (1,2790) | 1:7:A:THR:HA     | 1:20:A:GLN:H    | 4        | 0.15          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H    | 1        | 0.15          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H    | 3        | 0.15          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H    | 5        | 0.15          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H    | 7        | 0.15          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H    | 14       | 0.15          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H    | 18       | 0.15          |
| (1,2685) | 1:54:A:LEU:H     | 1:82:A:VAL:HB   | 10       | 0.15          |
| (1,2166) | 1:83:A:ILE:HG21  | 1:107:A:SER:H   | 15       | 0.15          |
| (1,2166) | 1:83:A:ILE:HG22  | 1:107:A:SER:H   | 15       | 0.15          |
| (1,2166) | 1:83:A:ILE:HG23  | 1:107:A:SER:H   | 15       | 0.15          |
| (1,2130) | 1:219:A:LEU:HD11 | 1:222:A:THR:HG1 | 20       | 0.15          |
| (1,2130) | 1:219:A:LEU:HD12 | 1:222:A:THR:HG1 | 20       | 0.15          |
| (1,2130) | 1:219:A:LEU:HD13 | 1:222:A:THR:HG1 | 20       | 0.15          |
| (1,1938) | 1:18:A:ILE:HA    | 1:19:A:SER:HA   | 10       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1447) | 1:190:A:SER:HB2  | 1:226:A:LEU:HB2  | 4        | 0.15          |
| (1,1447) | 1:190:A:SER:HB2  | 1:226:A:LEU:HB3  | 4        | 0.15          |
| (1,1447) | 1:190:A:SER:HB3  | 1:226:A:LEU:HB2  | 4        | 0.15          |
| (1,1447) | 1:190:A:SER:HB3  | 1:226:A:LEU:HB3  | 4        | 0.15          |
| (1,1160) | 1:175:A:ALA:HB1  | 1:221:A:HIS:HD2  | 11       | 0.15          |
| (1,1160) | 1:175:A:ALA:HB2  | 1:221:A:HIS:HD2  | 11       | 0.15          |
| (1,1160) | 1:175:A:ALA:HB3  | 1:221:A:HIS:HD2  | 11       | 0.15          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG21  | 15       | 0.15          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG22  | 15       | 0.15          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG23  | 15       | 0.15          |
| (1,773)  | 1:84:A:ILE:HD11  | 1:92:A:ILE:HB    | 15       | 0.15          |
| (1,773)  | 1:84:A:ILE:HD12  | 1:92:A:ILE:HB    | 15       | 0.15          |
| (1,773)  | 1:84:A:ILE:HD13  | 1:92:A:ILE:HB    | 15       | 0.15          |
| (1,370)  | 1:28:A:HIS:H     | 1:42:A:ASN:HA    | 7        | 0.15          |
| (1,370)  | 1:28:A:HIS:H     | 1:42:A:ASN:HA    | 9        | 0.15          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 3        | 0.15          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 3        | 0.15          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 3        | 0.15          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 3        | 0.15          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 3        | 0.15          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 3        | 0.15          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 3        | 0.15          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 3        | 0.15          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 3        | 0.15          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 9        | 0.15          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 9        | 0.15          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 9        | 0.15          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 9        | 0.15          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 9        | 0.15          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 9        | 0.15          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 9        | 0.15          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 9        | 0.15          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 9        | 0.15          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 13       | 0.15          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 13       | 0.15          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 13       | 0.15          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 13       | 0.15          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 13       | 0.15          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 13       | 0.15          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 13       | 0.15          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 13       | 0.15          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 13       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 15       | 0.15          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 15       | 0.15          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 15       | 0.15          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 15       | 0.15          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 15       | 0.15          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 15       | 0.15          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 15       | 0.15          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 15       | 0.15          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 15       | 0.15          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 3        | 0.15          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 3        | 0.15          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 3        | 0.15          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 6        | 0.15          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 6        | 0.15          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 6        | 0.15          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 15       | 0.15          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 15       | 0.15          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 15       | 0.15          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 18       | 0.15          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 18       | 0.15          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 18       | 0.15          |
| (3,1)    | 1:149:A:HIS:NE2  | 2:301:A:ZN:ZN    | 2        | 0.14          |
| (2,2)    | 1:218:A:LEU:HD11 | 1:221:A:HIS:HB2  | 11       | 0.14          |
| (2,2)    | 1:218:A:LEU:HD12 | 1:221:A:HIS:HB2  | 11       | 0.14          |
| (2,2)    | 1:218:A:LEU:HD13 | 1:221:A:HIS:HB2  | 11       | 0.14          |
| (1,5457) | 1:39:A:VAL:HG11  | 1:59:A:TRP:HE1   | 16       | 0.14          |
| (1,5457) | 1:39:A:VAL:HG12  | 1:59:A:TRP:HE1   | 16       | 0.14          |
| (1,5457) | 1:39:A:VAL:HG13  | 1:59:A:TRP:HE1   | 16       | 0.14          |
| (1,5457) | 1:39:A:VAL:HG21  | 1:59:A:TRP:HE1   | 16       | 0.14          |
| (1,5457) | 1:39:A:VAL:HG22  | 1:59:A:TRP:HE1   | 16       | 0.14          |
| (1,5457) | 1:39:A:VAL:HG23  | 1:59:A:TRP:HE1   | 16       | 0.14          |
| (1,5447) | 1:37:A:GLU:HB2   | 1:39:A:VAL:HG11  | 12       | 0.14          |
| (1,5447) | 1:37:A:GLU:HB2   | 1:39:A:VAL:HG12  | 12       | 0.14          |
| (1,5447) | 1:37:A:GLU:HB2   | 1:39:A:VAL:HG13  | 12       | 0.14          |
| (1,5447) | 1:37:A:GLU:HB2   | 1:39:A:VAL:HG21  | 12       | 0.14          |
| (1,5447) | 1:37:A:GLU:HB2   | 1:39:A:VAL:HG22  | 12       | 0.14          |
| (1,5447) | 1:37:A:GLU:HB2   | 1:39:A:VAL:HG23  | 12       | 0.14          |
| (1,4940) | 1:115:A:ALA:H    | 1:120:A:TYR:HD1  | 15       | 0.14          |
| (1,4940) | 1:115:A:ALA:H    | 1:120:A:TYR:HD2  | 15       | 0.14          |
| (1,4940) | 1:115:A:ALA:H    | 1:120:A:TYR:HD1  | 19       | 0.14          |
| (1,4940) | 1:115:A:ALA:H    | 1:120:A:TYR:HD2  | 19       | 0.14          |
| (1,4699) | 1:213:A:VAL:H    | 1:213:A:VAL:HB   | 11       | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,4675) | 1:208:A:PRO:HD3  | 1:210:A:HIS:H   | 7        | 0.14          |
| (1,4675) | 1:208:A:PRO:HD3  | 1:210:A:HIS:H   | 9        | 0.14          |
| (1,4675) | 1:208:A:PRO:HD3  | 1:210:A:HIS:H   | 16       | 0.14          |
| (1,4675) | 1:208:A:PRO:HD3  | 1:210:A:HIS:H   | 18       | 0.14          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H   | 2        | 0.14          |
| (1,4092) | 1:87:A:ALA:H     | 1:153:A:ASN:H   | 14       | 0.14          |
| (1,4092) | 1:87:A:ALA:H     | 1:153:A:ASN:H   | 18       | 0.14          |
| (1,3701) | 1:83:A:ILE:HA    | 1:107:A:SER:H   | 17       | 0.14          |
| (1,3572) | 1:95:A:ILE:H     | 1:120:A:TYR:HE1 | 19       | 0.14          |
| (1,3572) | 1:95:A:ILE:H     | 1:120:A:TYR:HE2 | 19       | 0.14          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 2        | 0.14          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 2        | 0.14          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 2        | 0.14          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 6        | 0.14          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 6        | 0.14          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 6        | 0.14          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 11       | 0.14          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 11       | 0.14          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 11       | 0.14          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 12       | 0.14          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 12       | 0.14          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 12       | 0.14          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 19       | 0.14          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 19       | 0.14          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 19       | 0.14          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H    | 8        | 0.14          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H    | 11       | 0.14          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H    | 20       | 0.14          |
| (1,3058) | 1:46:A:LEU:H     | 1:54:A:LEU:HB3  | 13       | 0.14          |
| (1,3058) | 1:46:A:LEU:H     | 1:54:A:LEU:HB3  | 20       | 0.14          |
| (1,2991) | 1:34:A:PHE:HD1   | 1:39:A:VAL:H    | 18       | 0.14          |
| (1,2991) | 1:34:A:PHE:HD2   | 1:39:A:VAL:H    | 18       | 0.14          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H    | 1        | 0.14          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H    | 3        | 0.14          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H    | 4        | 0.14          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H    | 6        | 0.14          |
| (1,2800) | 1:8:A:VAL:HB     | 1:20:A:GLN:H    | 6        | 0.14          |
| (1,2800) | 1:8:A:VAL:HB     | 1:20:A:GLN:H    | 9        | 0.14          |
| (1,2800) | 1:8:A:VAL:HB     | 1:20:A:GLN:H    | 18       | 0.14          |
| (1,2800) | 1:8:A:VAL:HB     | 1:20:A:GLN:H    | 20       | 0.14          |
| (1,2790) | 1:7:A:THR:HA     | 1:20:A:GLN:H    | 5        | 0.14          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H    | 4        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H     | 12       | 0.14          |
| (1,2775) | 1:9:A:ILE:HB     | 1:19:A:SER:H     | 16       | 0.14          |
| (1,2685) | 1:54:A:LEU:H     | 1:82:A:VAL:HB    | 6        | 0.14          |
| (1,2518) | 1:195:A:ASN:HB3  | 1:198:A:LYS:HB2  | 1        | 0.14          |
| (1,2518) | 1:195:A:ASN:HB3  | 1:198:A:LYS:HB3  | 1        | 0.14          |
| (1,2518) | 1:195:A:ASN:HB3  | 1:198:A:LYS:HB2  | 14       | 0.14          |
| (1,2518) | 1:195:A:ASN:HB3  | 1:198:A:LYS:HB3  | 14       | 0.14          |
| (1,2394) | 1:114:A:LEU:HB2  | 1:150:A:THR:HB   | 15       | 0.14          |
| (1,2130) | 1:219:A:LEU:HD11 | 1:222:A:THR:HG1  | 15       | 0.14          |
| (1,2130) | 1:219:A:LEU:HD12 | 1:222:A:THR:HG1  | 15       | 0.14          |
| (1,2130) | 1:219:A:LEU:HD13 | 1:222:A:THR:HG1  | 15       | 0.14          |
| (1,2097) | 1:58:A:SER:HB2   | 1:67:A:LEU:HG    | 16       | 0.14          |
| (1,2097) | 1:58:A:SER:HB2   | 1:67:A:LEU:HG    | 19       | 0.14          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG21  | 20       | 0.14          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG22  | 20       | 0.14          |
| (1,795)  | 1:57:A:SER:H     | 1:92:A:ILE:HG23  | 20       | 0.14          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 1        | 0.14          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 1        | 0.14          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 1        | 0.14          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 1        | 0.14          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 1        | 0.14          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 1        | 0.14          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 1        | 0.14          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 1        | 0.14          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 1        | 0.14          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 7        | 0.14          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 7        | 0.14          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 7        | 0.14          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 7        | 0.14          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 7        | 0.14          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 7        | 0.14          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 7        | 0.14          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 7        | 0.14          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 7        | 0.14          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 8        | 0.14          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 8        | 0.14          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 8        | 0.14          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 8        | 0.14          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 8        | 0.14          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 8        | 0.14          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 8        | 0.14          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 8        | 0.14          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,329) | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 8        | 0.14          |
| (1,329) | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 10       | 0.14          |
| (1,329) | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 10       | 0.14          |
| (1,329) | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 10       | 0.14          |
| (1,329) | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 10       | 0.14          |
| (1,329) | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 10       | 0.14          |
| (1,329) | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 10       | 0.14          |
| (1,329) | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 10       | 0.14          |
| (1,329) | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 10       | 0.14          |
| (1,329) | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 10       | 0.14          |
| (1,329) | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 14       | 0.14          |
| (1,329) | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 14       | 0.14          |
| (1,329) | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 14       | 0.14          |
| (1,329) | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 14       | 0.14          |
| (1,329) | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 14       | 0.14          |
| (1,329) | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 14       | 0.14          |
| (1,329) | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 14       | 0.14          |
| (1,329) | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 14       | 0.14          |
| (1,329) | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 14       | 0.14          |
| (1,329) | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 16       | 0.14          |
| (1,329) | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 16       | 0.14          |
| (1,329) | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 16       | 0.14          |
| (1,329) | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 16       | 0.14          |
| (1,329) | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 16       | 0.14          |
| (1,329) | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 16       | 0.14          |
| (1,329) | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 16       | 0.14          |
| (1,329) | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 16       | 0.14          |
| (1,329) | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 16       | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 2        | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 2        | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 2        | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 8        | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 8        | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 8        | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 11       | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 11       | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 11       | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 12       | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 12       | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 12       | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 14       | 0.14          |
| (1,150) | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 14       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 14       | 0.14          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 20       | 0.14          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 20       | 0.14          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 20       | 0.14          |
| (3,2)    | 1:168:A:CYS:SG   | 2:302:A:ZN:ZN    | 15       | 0.13          |
| (3,1)    | 1:149:A:HIS:NE2  | 2:301:A:ZN:ZN    | 7        | 0.13          |
| (2,9)    | 1:67:A:LEU:HD21  | 1:71:A:VAL:H     | 15       | 0.13          |
| (2,9)    | 1:67:A:LEU:HD22  | 1:71:A:VAL:H     | 15       | 0.13          |
| (2,9)    | 1:67:A:LEU:HD23  | 1:71:A:VAL:H     | 15       | 0.13          |
| (1,6437) | 1:178:A:LEU:H    | 1:226:A:LEU:HD11 | 11       | 0.13          |
| (1,6437) | 1:178:A:LEU:H    | 1:226:A:LEU:HD12 | 11       | 0.13          |
| (1,6437) | 1:178:A:LEU:H    | 1:226:A:LEU:HD13 | 11       | 0.13          |
| (1,6437) | 1:178:A:LEU:H    | 1:226:A:LEU:HD21 | 11       | 0.13          |
| (1,6437) | 1:178:A:LEU:H    | 1:226:A:LEU:HD22 | 11       | 0.13          |
| (1,6437) | 1:178:A:LEU:H    | 1:226:A:LEU:HD23 | 11       | 0.13          |
| (1,5671) | 1:54:A:LEU:HD11  | 1:55:A:VAL:H     | 3        | 0.13          |
| (1,5671) | 1:54:A:LEU:HD12  | 1:55:A:VAL:H     | 3        | 0.13          |
| (1,5671) | 1:54:A:LEU:HD13  | 1:55:A:VAL:H     | 3        | 0.13          |
| (1,5671) | 1:54:A:LEU:HD21  | 1:55:A:VAL:H     | 3        | 0.13          |
| (1,5671) | 1:54:A:LEU:HD22  | 1:55:A:VAL:H     | 3        | 0.13          |
| (1,5671) | 1:54:A:LEU:HD23  | 1:55:A:VAL:H     | 3        | 0.13          |
| (1,5457) | 1:39:A:VAL:HG11  | 1:59:A:TRP:HE1   | 3        | 0.13          |
| (1,5457) | 1:39:A:VAL:HG12  | 1:59:A:TRP:HE1   | 3        | 0.13          |
| (1,5457) | 1:39:A:VAL:HG13  | 1:59:A:TRP:HE1   | 3        | 0.13          |
| (1,5457) | 1:39:A:VAL:HG21  | 1:59:A:TRP:HE1   | 3        | 0.13          |
| (1,5457) | 1:39:A:VAL:HG22  | 1:59:A:TRP:HE1   | 3        | 0.13          |
| (1,5457) | 1:39:A:VAL:HG23  | 1:59:A:TRP:HE1   | 3        | 0.13          |
| (1,5457) | 1:39:A:VAL:HG11  | 1:59:A:TRP:HE1   | 6        | 0.13          |
| (1,5457) | 1:39:A:VAL:HG12  | 1:59:A:TRP:HE1   | 6        | 0.13          |
| (1,5457) | 1:39:A:VAL:HG13  | 1:59:A:TRP:HE1   | 6        | 0.13          |
| (1,5457) | 1:39:A:VAL:HG21  | 1:59:A:TRP:HE1   | 6        | 0.13          |
| (1,5457) | 1:39:A:VAL:HG22  | 1:59:A:TRP:HE1   | 6        | 0.13          |
| (1,5457) | 1:39:A:VAL:HG23  | 1:59:A:TRP:HE1   | 6        | 0.13          |
| (1,4940) | 1:115:A:ALA:H    | 1:120:A:TYR:HD1  | 20       | 0.13          |
| (1,4940) | 1:115:A:ALA:H    | 1:120:A:TYR:HD2  | 20       | 0.13          |
| (1,4675) | 1:208:A:PRO:HD3  | 1:210:A:HIS:H    | 4        | 0.13          |
| (1,4675) | 1:208:A:PRO:HD3  | 1:210:A:HIS:H    | 8        | 0.13          |
| (1,4675) | 1:208:A:PRO:HD3  | 1:210:A:HIS:H    | 14       | 0.13          |
| (1,4675) | 1:208:A:PRO:HD3  | 1:210:A:HIS:H    | 20       | 0.13          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H    | 7        | 0.13          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H    | 10       | 0.13          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H    | 20       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,4092) | 1:87:A:ALA:H    | 1:153:A:ASN:H   | 4        | 0.13          |
| (1,4092) | 1:87:A:ALA:H    | 1:153:A:ASN:H   | 7        | 0.13          |
| (1,4092) | 1:87:A:ALA:H    | 1:153:A:ASN:H   | 20       | 0.13          |
| (1,3777) | 1:108:A:THR:HA  | 1:112:A:ALA:H   | 3        | 0.13          |
| (1,3572) | 1:95:A:ILE:H    | 1:120:A:TYR:HE1 | 17       | 0.13          |
| (1,3572) | 1:95:A:ILE:H    | 1:120:A:TYR:HE2 | 17       | 0.13          |
| (1,3413) | 1:68:A:ILE:HD11 | 1:79:A:VAL:H    | 3        | 0.13          |
| (1,3413) | 1:68:A:ILE:HD12 | 1:79:A:VAL:H    | 3        | 0.13          |
| (1,3413) | 1:68:A:ILE:HD13 | 1:79:A:VAL:H    | 3        | 0.13          |
| (1,3413) | 1:68:A:ILE:HD11 | 1:79:A:VAL:H    | 17       | 0.13          |
| (1,3413) | 1:68:A:ILE:HD12 | 1:79:A:VAL:H    | 17       | 0.13          |
| (1,3413) | 1:68:A:ILE:HD13 | 1:79:A:VAL:H    | 17       | 0.13          |
| (1,3196) | 1:30:A:GLU:HA   | 1:59:A:TRP:HE1  | 12       | 0.13          |
| (1,3173) | 1:58:A:SER:H    | 1:95:A:ILE:H    | 16       | 0.13          |
| (1,3170) | 1:57:A:SER:H    | 1:84:A:ILE:HA   | 20       | 0.13          |
| (1,3163) | 1:54:A:LEU:HA   | 1:56:A:ASP:H    | 2        | 0.13          |
| (1,2984) | 1:33:A:SER:HA   | 1:37:A:GLU:H    | 19       | 0.13          |
| (1,2963) | 1:32:A:GLY:HA2  | 1:33:A:SER:H    | 7        | 0.13          |
| (1,2892) | 1:37:A:GLU:HB3  | 1:38:A:ALA:H    | 12       | 0.13          |
| (1,2892) | 1:37:A:GLU:HB2  | 1:38:A:ALA:H    | 12       | 0.13          |
| (1,2842) | 1:20:A:GLN:HA   | 1:25:A:VAL:H    | 7        | 0.13          |
| (1,2842) | 1:20:A:GLN:HA   | 1:25:A:VAL:H    | 16       | 0.13          |
| (1,2842) | 1:20:A:GLN:HA   | 1:25:A:VAL:H    | 19       | 0.13          |
| (1,2800) | 1:8:A:VAL:HB    | 1:20:A:GLN:H    | 2        | 0.13          |
| (1,2800) | 1:8:A:VAL:HB    | 1:20:A:GLN:H    | 15       | 0.13          |
| (1,2800) | 1:8:A:VAL:HB    | 1:20:A:GLN:H    | 17       | 0.13          |
| (1,2790) | 1:7:A:THR:HA    | 1:20:A:GLN:H    | 7        | 0.13          |
| (1,2790) | 1:7:A:THR:HA    | 1:20:A:GLN:H    | 11       | 0.13          |
| (1,2790) | 1:7:A:THR:HA    | 1:20:A:GLN:H    | 13       | 0.13          |
| (1,2790) | 1:7:A:THR:HA    | 1:20:A:GLN:H    | 16       | 0.13          |
| (1,2790) | 1:7:A:THR:HA    | 1:20:A:GLN:H    | 19       | 0.13          |
| (1,2685) | 1:54:A:LEU:H    | 1:82:A:VAL:HB   | 4        | 0.13          |
| (1,2685) | 1:54:A:LEU:H    | 1:82:A:VAL:HB   | 5        | 0.13          |
| (1,2685) | 1:54:A:LEU:H    | 1:82:A:VAL:HB   | 9        | 0.13          |
| (1,2685) | 1:54:A:LEU:H    | 1:82:A:VAL:HB   | 11       | 0.13          |
| (1,2685) | 1:54:A:LEU:H    | 1:82:A:VAL:HB   | 14       | 0.13          |
| (1,2618) | 1:57:A:SER:HA   | 1:91:A:ARG:HA   | 18       | 0.13          |
| (1,2518) | 1:195:A:ASN:HB3 | 1:198:A:LYS:HB2 | 5        | 0.13          |
| (1,2518) | 1:195:A:ASN:HB3 | 1:198:A:LYS:HB3 | 5        | 0.13          |
| (1,2518) | 1:195:A:ASN:HB3 | 1:198:A:LYS:HB2 | 16       | 0.13          |
| (1,2518) | 1:195:A:ASN:HB3 | 1:198:A:LYS:HB3 | 16       | 0.13          |
| (1,2504) | 1:192:A:SER:HB3 | 1:195:A:ASN:H   | 10       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD11  | 14       | 0.13          |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD12  | 14       | 0.13          |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD13  | 14       | 0.13          |
| (1,1209) | 1:196:A:VAL:HA   | 1:219:A:LEU:HD21 | 9        | 0.13          |
| (1,1209) | 1:196:A:VAL:HA   | 1:219:A:LEU:HD22 | 9        | 0.13          |
| (1,1209) | 1:196:A:VAL:HA   | 1:219:A:LEU:HD23 | 9        | 0.13          |
| (1,1209) | 1:196:A:VAL:HA   | 1:219:A:LEU:HD21 | 11       | 0.13          |
| (1,1209) | 1:196:A:VAL:HA   | 1:219:A:LEU:HD22 | 11       | 0.13          |
| (1,1209) | 1:196:A:VAL:HA   | 1:219:A:LEU:HD23 | 11       | 0.13          |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB1  | 15       | 0.13          |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB2  | 15       | 0.13          |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB3  | 15       | 0.13          |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB1  | 17       | 0.13          |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB2  | 17       | 0.13          |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB3  | 17       | 0.13          |
| (1,773)  | 1:84:A:ILE:HD11  | 1:92:A:ILE:HB    | 16       | 0.13          |
| (1,773)  | 1:84:A:ILE:HD12  | 1:92:A:ILE:HB    | 16       | 0.13          |
| (1,773)  | 1:84:A:ILE:HD13  | 1:92:A:ILE:HB    | 16       | 0.13          |
| (1,773)  | 1:84:A:ILE:HD11  | 1:92:A:ILE:HB    | 17       | 0.13          |
| (1,773)  | 1:84:A:ILE:HD12  | 1:92:A:ILE:HB    | 17       | 0.13          |
| (1,773)  | 1:84:A:ILE:HD13  | 1:92:A:ILE:HB    | 17       | 0.13          |
| (1,773)  | 1:84:A:ILE:HD11  | 1:92:A:ILE:HB    | 19       | 0.13          |
| (1,773)  | 1:84:A:ILE:HD12  | 1:92:A:ILE:HB    | 19       | 0.13          |
| (1,773)  | 1:84:A:ILE:HD13  | 1:92:A:ILE:HB    | 19       | 0.13          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 17       | 0.13          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 17       | 0.13          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 17       | 0.13          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 17       | 0.13          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 17       | 0.13          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 17       | 0.13          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 17       | 0.13          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 17       | 0.13          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 17       | 0.13          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 18       | 0.13          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 18       | 0.13          |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 18       | 0.13          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 18       | 0.13          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 18       | 0.13          |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 18       | 0.13          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 18       | 0.13          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 18       | 0.13          |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 18       | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG21  | 1        | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG22  | 1        | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG23  | 1        | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG21  | 7        | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG22  | 7        | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG23  | 7        | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG21  | 9        | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG22  | 9        | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG23  | 9        | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG21  | 10       | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG22  | 10       | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG23  | 10       | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG21  | 13       | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG22  | 13       | 0.13          |
| (1,150)  | 1:14:A:GLY:H    | 1:15:A:THR:HG23  | 13       | 0.13          |
| (2,6)    | 1:32:A:GLY:H    | 1:40:A:PRO:HB2   | 9        | 0.12          |
| (1,6722) | 1:227:A:LYS:H   | 1:227:A:LYS:HG2  | 18       | 0.12          |
| (1,6722) | 1:227:A:LYS:H   | 1:227:A:LYS:HG3  | 18       | 0.12          |
| (1,6397) | 1:172:A:SER:HB2 | 1:173:A:THR:HG21 | 11       | 0.12          |
| (1,6397) | 1:172:A:SER:HB2 | 1:173:A:THR:HG22 | 11       | 0.12          |
| (1,6397) | 1:172:A:SER:HB2 | 1:173:A:THR:HG23 | 11       | 0.12          |
| (1,6397) | 1:172:A:SER:HB3 | 1:173:A:THR:HG21 | 11       | 0.12          |
| (1,6397) | 1:172:A:SER:HB3 | 1:173:A:THR:HG22 | 11       | 0.12          |
| (1,6397) | 1:172:A:SER:HB3 | 1:173:A:THR:HG23 | 11       | 0.12          |
| (1,5703) | 1:57:A:SER:HB2  | 1:64:A:THR:HB    | 16       | 0.12          |
| (1,5703) | 1:57:A:SER:HB3  | 1:64:A:THR:HB    | 16       | 0.12          |
| (1,5671) | 1:54:A:LEU:HD11 | 1:55:A:VAL:H     | 12       | 0.12          |
| (1,5671) | 1:54:A:LEU:HD12 | 1:55:A:VAL:H     | 12       | 0.12          |
| (1,5671) | 1:54:A:LEU:HD13 | 1:55:A:VAL:H     | 12       | 0.12          |
| (1,5671) | 1:54:A:LEU:HD21 | 1:55:A:VAL:H     | 12       | 0.12          |
| (1,5671) | 1:54:A:LEU:HD22 | 1:55:A:VAL:H     | 12       | 0.12          |
| (1,5671) | 1:54:A:LEU:HD23 | 1:55:A:VAL:H     | 12       | 0.12          |
| (1,5671) | 1:54:A:LEU:HD11 | 1:55:A:VAL:H     | 20       | 0.12          |
| (1,5671) | 1:54:A:LEU:HD12 | 1:55:A:VAL:H     | 20       | 0.12          |
| (1,5671) | 1:54:A:LEU:HD13 | 1:55:A:VAL:H     | 20       | 0.12          |
| (1,5671) | 1:54:A:LEU:HD21 | 1:55:A:VAL:H     | 20       | 0.12          |
| (1,5671) | 1:54:A:LEU:HD22 | 1:55:A:VAL:H     | 20       | 0.12          |
| (1,5671) | 1:54:A:LEU:HD23 | 1:55:A:VAL:H     | 20       | 0.12          |
| (1,5457) | 1:39:A:VAL:HG11 | 1:59:A:TRP:HE1   | 5        | 0.12          |
| (1,5457) | 1:39:A:VAL:HG12 | 1:59:A:TRP:HE1   | 5        | 0.12          |
| (1,5457) | 1:39:A:VAL:HG13 | 1:59:A:TRP:HE1   | 5        | 0.12          |
| (1,5457) | 1:39:A:VAL:HG21 | 1:59:A:TRP:HE1   | 5        | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,5457) | 1:39:A:VAL:HG22  | 1:59:A:TRP:HE1  | 5        | 0.12          |
| (1,5457) | 1:39:A:VAL:HG23  | 1:59:A:TRP:HE1  | 5        | 0.12          |
| (1,5457) | 1:39:A:VAL:HG11  | 1:59:A:TRP:HE1  | 7        | 0.12          |
| (1,5457) | 1:39:A:VAL:HG12  | 1:59:A:TRP:HE1  | 7        | 0.12          |
| (1,5457) | 1:39:A:VAL:HG13  | 1:59:A:TRP:HE1  | 7        | 0.12          |
| (1,5457) | 1:39:A:VAL:HG21  | 1:59:A:TRP:HE1  | 7        | 0.12          |
| (1,5457) | 1:39:A:VAL:HG22  | 1:59:A:TRP:HE1  | 7        | 0.12          |
| (1,5457) | 1:39:A:VAL:HG23  | 1:59:A:TRP:HE1  | 7        | 0.12          |
| (1,5457) | 1:39:A:VAL:HG11  | 1:59:A:TRP:HE1  | 18       | 0.12          |
| (1,5457) | 1:39:A:VAL:HG12  | 1:59:A:TRP:HE1  | 18       | 0.12          |
| (1,5457) | 1:39:A:VAL:HG13  | 1:59:A:TRP:HE1  | 18       | 0.12          |
| (1,5457) | 1:39:A:VAL:HG21  | 1:59:A:TRP:HE1  | 18       | 0.12          |
| (1,5457) | 1:39:A:VAL:HG22  | 1:59:A:TRP:HE1  | 18       | 0.12          |
| (1,5457) | 1:39:A:VAL:HG23  | 1:59:A:TRP:HE1  | 18       | 0.12          |
| (1,5440) | 1:35:A:ASN:HD21  | 1:39:A:VAL:HG11 | 17       | 0.12          |
| (1,5440) | 1:35:A:ASN:HD21  | 1:39:A:VAL:HG12 | 17       | 0.12          |
| (1,5440) | 1:35:A:ASN:HD21  | 1:39:A:VAL:HG13 | 17       | 0.12          |
| (1,5440) | 1:35:A:ASN:HD21  | 1:39:A:VAL:HG21 | 17       | 0.12          |
| (1,5440) | 1:35:A:ASN:HD21  | 1:39:A:VAL:HG22 | 17       | 0.12          |
| (1,5440) | 1:35:A:ASN:HD21  | 1:39:A:VAL:HG23 | 17       | 0.12          |
| (1,4954) | 1:81:A:ASP:HB2   | 1:106:A:HIS:HD2 | 18       | 0.12          |
| (1,4954) | 1:81:A:ASP:HB3   | 1:106:A:HIS:HD2 | 18       | 0.12          |
| (1,4699) | 1:213:A:VAL:H    | 1:213:A:VAL:HB  | 3        | 0.12          |
| (1,4699) | 1:213:A:VAL:H    | 1:213:A:VAL:HB  | 4        | 0.12          |
| (1,4699) | 1:213:A:VAL:H    | 1:213:A:VAL:HB  | 6        | 0.12          |
| (1,4699) | 1:213:A:VAL:H    | 1:213:A:VAL:HB  | 7        | 0.12          |
| (1,4699) | 1:213:A:VAL:H    | 1:213:A:VAL:HB  | 8        | 0.12          |
| (1,4699) | 1:213:A:VAL:H    | 1:213:A:VAL:HB  | 10       | 0.12          |
| (1,4699) | 1:213:A:VAL:H    | 1:213:A:VAL:HB  | 12       | 0.12          |
| (1,4699) | 1:213:A:VAL:H    | 1:213:A:VAL:HB  | 14       | 0.12          |
| (1,4699) | 1:213:A:VAL:H    | 1:213:A:VAL:HB  | 16       | 0.12          |
| (1,4699) | 1:213:A:VAL:H    | 1:213:A:VAL:HB  | 17       | 0.12          |
| (1,4699) | 1:213:A:VAL:H    | 1:213:A:VAL:HB  | 18       | 0.12          |
| (1,4699) | 1:213:A:VAL:H    | 1:213:A:VAL:HB  | 20       | 0.12          |
| (1,4675) | 1:208:A:PRO:HD3  | 1:210:A:HIS:H   | 2        | 0.12          |
| (1,4566) | 1:222:A:THR:HB   | 1:226:A:LEU:H   | 12       | 0.12          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H   | 1        | 0.12          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H   | 14       | 0.12          |
| (1,4092) | 1:87:A:ALA:H     | 1:153:A:ASN:H   | 1        | 0.12          |
| (1,4092) | 1:87:A:ALA:H     | 1:153:A:ASN:H   | 9        | 0.12          |
| (1,4092) | 1:87:A:ALA:H     | 1:153:A:ASN:H   | 11       | 0.12          |
| (1,4092) | 1:87:A:ALA:H     | 1:153:A:ASN:H   | 12       | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,4092) | 1:87:A:ALA:H     | 1:153:A:ASN:H   | 17       | 0.12          |
| (1,4040) | 1:148:A:GLY:H    | 1:151:A:GLU:H   | 7        | 0.12          |
| (1,3701) | 1:83:A:ILE:HA    | 1:107:A:SER:H   | 19       | 0.12          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 4        | 0.12          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 4        | 0.12          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 4        | 0.12          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 5        | 0.12          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 5        | 0.12          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 5        | 0.12          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 7        | 0.12          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 7        | 0.12          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 7        | 0.12          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 10       | 0.12          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 10       | 0.12          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 10       | 0.12          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 13       | 0.12          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 13       | 0.12          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 13       | 0.12          |
| (1,3173) | 1:58:A:SER:H     | 1:95:A:ILE:H    | 15       | 0.12          |
| (1,3163) | 1:54:A:LEU:HA    | 1:56:A:ASP:H    | 16       | 0.12          |
| (1,3100) | 1:48:A:THR:H     | 1:51:A:GLY:HA2  | 20       | 0.12          |
| (1,2963) | 1:32:A:GLY:HA2   | 1:33:A:SER:H    | 9        | 0.12          |
| (1,2875) | 1:22:A:ASN:H     | 1:26:A:TRP:HE1  | 5        | 0.12          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H    | 5        | 0.12          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H    | 11       | 0.12          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H    | 12       | 0.12          |
| (1,2790) | 1:7:A:THR:HA     | 1:20:A:GLN:H    | 12       | 0.12          |
| (1,2685) | 1:54:A:LEU:H     | 1:82:A:VAL:HB   | 3        | 0.12          |
| (1,2685) | 1:54:A:LEU:H     | 1:82:A:VAL:HB   | 8        | 0.12          |
| (1,2685) | 1:54:A:LEU:H     | 1:82:A:VAL:HB   | 12       | 0.12          |
| (1,2618) | 1:57:A:SER:HA    | 1:91:A:ARG:HA   | 8        | 0.12          |
| (1,2618) | 1:57:A:SER:HA    | 1:91:A:ARG:HA   | 12       | 0.12          |
| (1,2518) | 1:195:A:ASN:HB3  | 1:198:A:LYS:HB2 | 4        | 0.12          |
| (1,2518) | 1:195:A:ASN:HB3  | 1:198:A:LYS:HB3 | 4        | 0.12          |
| (1,2518) | 1:195:A:ASN:HB3  | 1:198:A:LYS:HB2 | 13       | 0.12          |
| (1,2518) | 1:195:A:ASN:HB3  | 1:198:A:LYS:HB3 | 13       | 0.12          |
| (1,2518) | 1:195:A:ASN:HB3  | 1:198:A:LYS:HB2 | 18       | 0.12          |
| (1,2518) | 1:195:A:ASN:HB3  | 1:198:A:LYS:HB3 | 18       | 0.12          |
| (1,2130) | 1:219:A:LEU:HD11 | 1:222:A:THR:HG1 | 2        | 0.12          |
| (1,2130) | 1:219:A:LEU:HD12 | 1:222:A:THR:HG1 | 2        | 0.12          |
| (1,2130) | 1:219:A:LEU:HD13 | 1:222:A:THR:HG1 | 2        | 0.12          |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD11 | 16       | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2109) | 1:67:A:LEU:H    | 1:68:A:ILE:HD12  | 16       | 0.12          |
| (1,2109) | 1:67:A:LEU:H    | 1:68:A:ILE:HD13  | 16       | 0.12          |
| (1,2097) | 1:58:A:SER:HB2  | 1:67:A:LEU:HG    | 7        | 0.12          |
| (1,2097) | 1:58:A:SER:HB2  | 1:67:A:LEU:HG    | 14       | 0.12          |
| (1,1981) | 1:33:A:SER:HB3  | 1:38:A:ALA:HB1   | 18       | 0.12          |
| (1,1981) | 1:33:A:SER:HB3  | 1:38:A:ALA:HB2   | 18       | 0.12          |
| (1,1981) | 1:33:A:SER:HB3  | 1:38:A:ALA:HB3   | 18       | 0.12          |
| (1,1463) | 1:190:A:SER:HA  | 1:226:A:LEU:HB2  | 7        | 0.12          |
| (1,1463) | 1:190:A:SER:HA  | 1:226:A:LEU:HB3  | 7        | 0.12          |
| (1,1406) | 1:84:A:ILE:HG21 | 1:91:A:ARG:HA    | 16       | 0.12          |
| (1,1406) | 1:84:A:ILE:HG22 | 1:91:A:ARG:HA    | 16       | 0.12          |
| (1,1406) | 1:84:A:ILE:HG23 | 1:91:A:ARG:HA    | 16       | 0.12          |
| (1,1406) | 1:84:A:ILE:HG21 | 1:91:A:ARG:HA    | 19       | 0.12          |
| (1,1406) | 1:84:A:ILE:HG22 | 1:91:A:ARG:HA    | 19       | 0.12          |
| (1,1406) | 1:84:A:ILE:HG23 | 1:91:A:ARG:HA    | 19       | 0.12          |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD21 | 4        | 0.12          |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD22 | 4        | 0.12          |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD23 | 4        | 0.12          |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD21 | 5        | 0.12          |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD22 | 5        | 0.12          |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD23 | 5        | 0.12          |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD21 | 12       | 0.12          |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD22 | 12       | 0.12          |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD23 | 12       | 0.12          |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD21 | 16       | 0.12          |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD22 | 16       | 0.12          |
| (1,1209) | 1:196:A:VAL:HA  | 1:219:A:LEU:HD23 | 16       | 0.12          |
| (1,899)  | 1:109:A:ALA:HB1 | 1:113:A:GLU:H    | 18       | 0.12          |
| (1,899)  | 1:109:A:ALA:HB2 | 1:113:A:GLU:H    | 18       | 0.12          |
| (1,899)  | 1:109:A:ALA:HB3 | 1:113:A:GLU:H    | 18       | 0.12          |
| (1,867)  | 1:57:A:SER:H    | 1:105:A:ALA:HB1  | 19       | 0.12          |
| (1,867)  | 1:57:A:SER:H    | 1:105:A:ALA:HB2  | 19       | 0.12          |
| (1,867)  | 1:57:A:SER:H    | 1:105:A:ALA:HB3  | 19       | 0.12          |
| (1,773)  | 1:84:A:ILE:HD11 | 1:92:A:ILE:HB    | 20       | 0.12          |
| (1,773)  | 1:84:A:ILE:HD12 | 1:92:A:ILE:HB    | 20       | 0.12          |
| (1,773)  | 1:84:A:ILE:HD13 | 1:92:A:ILE:HB    | 20       | 0.12          |
| (1,666)  | 1:68:A:ILE:HG21 | 1:78:A:ARG:HB2   | 9        | 0.12          |
| (1,666)  | 1:68:A:ILE:HG21 | 1:78:A:ARG:HB3   | 9        | 0.12          |
| (1,666)  | 1:68:A:ILE:HG22 | 1:78:A:ARG:HB2   | 9        | 0.12          |
| (1,666)  | 1:68:A:ILE:HG22 | 1:78:A:ARG:HB3   | 9        | 0.12          |
| (1,666)  | 1:68:A:ILE:HG23 | 1:78:A:ARG:HB2   | 9        | 0.12          |
| (1,666)  | 1:68:A:ILE:HG23 | 1:78:A:ARG:HB3   | 9        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,317)  | 1:186:A:VAL:HG21 | 1:187:A:ASN:HB2  | 18       | 0.12          |
| (1,317)  | 1:186:A:VAL:HG21 | 1:187:A:ASN:HB3  | 18       | 0.12          |
| (1,317)  | 1:186:A:VAL:HG22 | 1:187:A:ASN:HB2  | 18       | 0.12          |
| (1,317)  | 1:186:A:VAL:HG22 | 1:187:A:ASN:HB3  | 18       | 0.12          |
| (1,317)  | 1:186:A:VAL:HG23 | 1:187:A:ASN:HB2  | 18       | 0.12          |
| (1,317)  | 1:186:A:VAL:HG23 | 1:187:A:ASN:HB3  | 18       | 0.12          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 4        | 0.12          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 4        | 0.12          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 4        | 0.12          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 5        | 0.12          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 5        | 0.12          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 5        | 0.12          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG21  | 16       | 0.12          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG22  | 16       | 0.12          |
| (1,150)  | 1:14:A:GLY:H     | 1:15:A:THR:HG23  | 16       | 0.12          |
| (1,39)   | 1:34:A:PHE:HD1   | 1:39:A:VAL:HB    | 10       | 0.12          |
| (1,39)   | 1:34:A:PHE:HD2   | 1:39:A:VAL:HB    | 10       | 0.12          |
| (3,1)    | 1:149:A:HIS:NE2  | 2:301:A:ZN:ZN    | 13       | 0.11          |
| (3,1)    | 1:149:A:HIS:NE2  | 2:301:A:ZN:ZN    | 15       | 0.11          |
| (2,7)    | 1:218:A:LEU:H    | 1:219:A:LEU:HG   | 11       | 0.11          |
| (1,6691) | 1:222:A:THR:HA   | 1:223:A:LEU:HD11 | 19       | 0.11          |
| (1,6691) | 1:222:A:THR:HA   | 1:223:A:LEU:HD12 | 19       | 0.11          |
| (1,6691) | 1:222:A:THR:HA   | 1:223:A:LEU:HD13 | 19       | 0.11          |
| (1,6691) | 1:222:A:THR:HA   | 1:223:A:LEU:HD21 | 19       | 0.11          |
| (1,6691) | 1:222:A:THR:HA   | 1:223:A:LEU:HD22 | 19       | 0.11          |
| (1,6691) | 1:222:A:THR:HA   | 1:223:A:LEU:HD23 | 19       | 0.11          |
| (1,6408) | 1:173:A:THR:HB   | 1:218:A:LEU:HD11 | 11       | 0.11          |
| (1,6408) | 1:173:A:THR:HB   | 1:218:A:LEU:HD12 | 11       | 0.11          |
| (1,6408) | 1:173:A:THR:HB   | 1:218:A:LEU:HD13 | 11       | 0.11          |
| (1,6408) | 1:173:A:THR:HB   | 1:218:A:LEU:HD21 | 11       | 0.11          |
| (1,6408) | 1:173:A:THR:HB   | 1:218:A:LEU:HD22 | 11       | 0.11          |
| (1,6408) | 1:173:A:THR:HB   | 1:218:A:LEU:HD23 | 11       | 0.11          |
| (1,6388) | 1:171:A:LYS:HB2  | 1:175:A:ALA:H    | 11       | 0.11          |
| (1,6388) | 1:171:A:LYS:HB3  | 1:175:A:ALA:H    | 11       | 0.11          |
| (1,5893) | 1:95:A:ILE:HG12  | 1:121:A:GLU:HB2  | 18       | 0.11          |
| (1,5893) | 1:95:A:ILE:HG12  | 1:121:A:GLU:HB3  | 18       | 0.11          |
| (1,5671) | 1:54:A:LEU:HD11  | 1:55:A:VAL:H     | 5        | 0.11          |
| (1,5671) | 1:54:A:LEU:HD12  | 1:55:A:VAL:H     | 5        | 0.11          |
| (1,5671) | 1:54:A:LEU:HD13  | 1:55:A:VAL:H     | 5        | 0.11          |
| (1,5671) | 1:54:A:LEU:HD21  | 1:55:A:VAL:H     | 5        | 0.11          |
| (1,5671) | 1:54:A:LEU:HD22  | 1:55:A:VAL:H     | 5        | 0.11          |
| (1,5671) | 1:54:A:LEU:HD23  | 1:55:A:VAL:H     | 5        | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,5217) | 1:8:A:VAL:HG11   | 1:17:A:SER:HA   | 10       | 0.11          |
| (1,5217) | 1:8:A:VAL:HG12   | 1:17:A:SER:HA   | 10       | 0.11          |
| (1,5217) | 1:8:A:VAL:HG13   | 1:17:A:SER:HA   | 10       | 0.11          |
| (1,5217) | 1:8:A:VAL:HG21   | 1:17:A:SER:HA   | 10       | 0.11          |
| (1,5217) | 1:8:A:VAL:HG22   | 1:17:A:SER:HA   | 10       | 0.11          |
| (1,5217) | 1:8:A:VAL:HG23   | 1:17:A:SER:HA   | 10       | 0.11          |
| (1,4796) | 1:222:A:THR:HG1  | 1:224:A:ASP:H   | 7        | 0.11          |
| (1,4796) | 1:222:A:THR:HG1  | 1:224:A:ASP:H   | 11       | 0.11          |
| (1,4796) | 1:222:A:THR:HG1  | 1:224:A:ASP:H   | 19       | 0.11          |
| (1,4675) | 1:208:A:PRO:HD3  | 1:210:A:HIS:H   | 6        | 0.11          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H   | 4        | 0.11          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H   | 5        | 0.11          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H   | 6        | 0.11          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H   | 13       | 0.11          |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H   | 16       | 0.11          |
| (1,4319) | 1:177:A:ASP:HB2  | 1:178:A:LEU:H   | 3        | 0.11          |
| (1,4265) | 1:170:A:VAL:H    | 1:222:A:THR:HG1 | 11       | 0.11          |
| (1,4040) | 1:148:A:GLY:H    | 1:151:A:GLU:H   | 14       | 0.11          |
| (1,4040) | 1:148:A:GLY:H    | 1:151:A:GLU:H   | 16       | 0.11          |
| (1,4040) | 1:148:A:GLY:H    | 1:151:A:GLU:H   | 17       | 0.11          |
| (1,4040) | 1:148:A:GLY:H    | 1:151:A:GLU:H   | 18       | 0.11          |
| (1,4040) | 1:148:A:GLY:H    | 1:151:A:GLU:H   | 20       | 0.11          |
| (1,3799) | 1:113:A:GLU:HB2  | 1:116:A:LYS:H   | 12       | 0.11          |
| (1,3799) | 1:113:A:GLU:HB3  | 1:116:A:LYS:H   | 12       | 0.11          |
| (1,3799) | 1:113:A:GLU:HB2  | 1:116:A:LYS:H   | 13       | 0.11          |
| (1,3799) | 1:113:A:GLU:HB3  | 1:116:A:LYS:H   | 13       | 0.11          |
| (1,3799) | 1:113:A:GLU:HB2  | 1:116:A:LYS:H   | 19       | 0.11          |
| (1,3799) | 1:113:A:GLU:HB3  | 1:116:A:LYS:H   | 19       | 0.11          |
| (1,3749) | 1:110:A:LEU:HB2  | 1:111:A:THR:H   | 20       | 0.11          |
| (1,3701) | 1:83:A:ILE:HA    | 1:107:A:SER:H   | 16       | 0.11          |
| (1,3701) | 1:83:A:ILE:HA    | 1:107:A:SER:H   | 20       | 0.11          |
| (1,3572) | 1:95:A:ILE:H     | 1:120:A:TYR:HE1 | 20       | 0.11          |
| (1,3572) | 1:95:A:ILE:H     | 1:120:A:TYR:HE2 | 20       | 0.11          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 1        | 0.11          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 1        | 0.11          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 1        | 0.11          |
| (1,3413) | 1:68:A:ILE:HD11  | 1:79:A:VAL:H    | 18       | 0.11          |
| (1,3413) | 1:68:A:ILE:HD12  | 1:79:A:VAL:H    | 18       | 0.11          |
| (1,3413) | 1:68:A:ILE:HD13  | 1:79:A:VAL:H    | 18       | 0.11          |
| (1,3173) | 1:58:A:SER:H     | 1:95:A:ILE:H    | 19       | 0.11          |
| (1,3168) | 1:56:A:ASP:H     | 1:57:A:SER:H    | 15       | 0.11          |
| (1,3168) | 1:56:A:ASP:H     | 1:57:A:SER:H    | 16       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3158) | 1:56:A:ASP:H     | 1:82:A:VAL:HB    | 15       | 0.11          |
| (1,3130) | 1:52:A:LEU:H     | 1:81:A:ASP:H     | 13       | 0.11          |
| (1,3058) | 1:46:A:LEU:H     | 1:54:A:LEU:HB3   | 2        | 0.11          |
| (1,3058) | 1:46:A:LEU:H     | 1:54:A:LEU:HB3   | 9        | 0.11          |
| (1,3058) | 1:46:A:LEU:H     | 1:54:A:LEU:HB3   | 14       | 0.11          |
| (1,2842) | 1:20:A:GLN:HA    | 1:25:A:VAL:H     | 13       | 0.11          |
| (1,2685) | 1:54:A:LEU:H     | 1:82:A:VAL:HB    | 1        | 0.11          |
| (1,2685) | 1:54:A:LEU:H     | 1:82:A:VAL:HB    | 2        | 0.11          |
| (1,2685) | 1:54:A:LEU:H     | 1:82:A:VAL:HB    | 7        | 0.11          |
| (1,2623) | 1:135:A:PHE:HA   | 1:138:A:MET:HG2  | 13       | 0.11          |
| (1,2623) | 1:135:A:PHE:HA   | 1:138:A:MET:HG3  | 13       | 0.11          |
| (1,2618) | 1:57:A:SER:HA    | 1:91:A:ARG:HA    | 3        | 0.11          |
| (1,2591) | 1:196:A:VAL:HA   | 1:219:A:LEU:HD11 | 19       | 0.11          |
| (1,2591) | 1:196:A:VAL:HA   | 1:219:A:LEU:HD12 | 19       | 0.11          |
| (1,2591) | 1:196:A:VAL:HA   | 1:219:A:LEU:HD13 | 19       | 0.11          |
| (1,2583) | 1:172:A:SER:HA   | 1:218:A:LEU:HA   | 11       | 0.11          |
| (1,2518) | 1:195:A:ASN:HB3  | 1:198:A:LYS:HB2  | 6        | 0.11          |
| (1,2518) | 1:195:A:ASN:HB3  | 1:198:A:LYS:HB3  | 6        | 0.11          |
| (1,2256) | 1:87:A:ALA:HB1   | 1:151:A:GLU:H    | 10       | 0.11          |
| (1,2256) | 1:87:A:ALA:HB2   | 1:151:A:GLU:H    | 10       | 0.11          |
| (1,2256) | 1:87:A:ALA:HB3   | 1:151:A:GLU:H    | 10       | 0.11          |
| (1,2249) | 1:110:A:LEU:HG   | 1:111:A:THR:HA   | 8        | 0.11          |
| (1,2190) | 1:89:A:ALA:HB1   | 1:120:A:TYR:HD1  | 16       | 0.11          |
| (1,2190) | 1:89:A:ALA:HB1   | 1:120:A:TYR:HD2  | 16       | 0.11          |
| (1,2190) | 1:89:A:ALA:HB2   | 1:120:A:TYR:HD1  | 16       | 0.11          |
| (1,2190) | 1:89:A:ALA:HB2   | 1:120:A:TYR:HD2  | 16       | 0.11          |
| (1,2190) | 1:89:A:ALA:HB3   | 1:120:A:TYR:HD1  | 16       | 0.11          |
| (1,2190) | 1:89:A:ALA:HB3   | 1:120:A:TYR:HD2  | 16       | 0.11          |
| (1,2168) | 1:84:A:ILE:HA    | 1:91:A:ARG:HA    | 19       | 0.11          |
| (1,2166) | 1:83:A:ILE:HG21  | 1:107:A:SER:H    | 16       | 0.11          |
| (1,2166) | 1:83:A:ILE:HG22  | 1:107:A:SER:H    | 16       | 0.11          |
| (1,2166) | 1:83:A:ILE:HG23  | 1:107:A:SER:H    | 16       | 0.11          |
| (1,2166) | 1:83:A:ILE:HG21  | 1:107:A:SER:H    | 17       | 0.11          |
| (1,2166) | 1:83:A:ILE:HG22  | 1:107:A:SER:H    | 17       | 0.11          |
| (1,2166) | 1:83:A:ILE:HG23  | 1:107:A:SER:H    | 17       | 0.11          |
| (1,2166) | 1:83:A:ILE:HG21  | 1:107:A:SER:H    | 19       | 0.11          |
| (1,2166) | 1:83:A:ILE:HG22  | 1:107:A:SER:H    | 19       | 0.11          |
| (1,2166) | 1:83:A:ILE:HG23  | 1:107:A:SER:H    | 19       | 0.11          |
| (1,2130) | 1:219:A:LEU:HD11 | 1:222:A:THR:HG1  | 19       | 0.11          |
| (1,2130) | 1:219:A:LEU:HD12 | 1:222:A:THR:HG1  | 19       | 0.11          |
| (1,2130) | 1:219:A:LEU:HD13 | 1:222:A:THR:HG1  | 19       | 0.11          |
| (1,2097) | 1:58:A:SER:HB2   | 1:67:A:LEU:HG    | 4        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2097) | 1:58:A:SER:HB2   | 1:67:A:LEU:HG    | 12       | 0.11          |
| (1,2097) | 1:58:A:SER:HB2   | 1:67:A:LEU:HG    | 17       | 0.11          |
| (1,1463) | 1:190:A:SER:HA   | 1:226:A:LEU:HB2  | 5        | 0.11          |
| (1,1463) | 1:190:A:SER:HA   | 1:226:A:LEU:HB3  | 5        | 0.11          |
| (1,1406) | 1:84:A:ILE:HG21  | 1:91:A:ARG:HA    | 15       | 0.11          |
| (1,1406) | 1:84:A:ILE:HG22  | 1:91:A:ARG:HA    | 15       | 0.11          |
| (1,1406) | 1:84:A:ILE:HG23  | 1:91:A:ARG:HA    | 15       | 0.11          |
| (1,1406) | 1:84:A:ILE:HG21  | 1:91:A:ARG:HA    | 17       | 0.11          |
| (1,1406) | 1:84:A:ILE:HG22  | 1:91:A:ARG:HA    | 17       | 0.11          |
| (1,1406) | 1:84:A:ILE:HG23  | 1:91:A:ARG:HA    | 17       | 0.11          |
| (1,1209) | 1:196:A:VAL:HA   | 1:219:A:LEU:HD21 | 8        | 0.11          |
| (1,1209) | 1:196:A:VAL:HA   | 1:219:A:LEU:HD22 | 8        | 0.11          |
| (1,1209) | 1:196:A:VAL:HA   | 1:219:A:LEU:HD23 | 8        | 0.11          |
| (1,899)  | 1:109:A:ALA:HB1  | 1:113:A:GLU:H    | 13       | 0.11          |
| (1,899)  | 1:109:A:ALA:HB2  | 1:113:A:GLU:H    | 13       | 0.11          |
| (1,899)  | 1:109:A:ALA:HB3  | 1:113:A:GLU:H    | 13       | 0.11          |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB1  | 20       | 0.11          |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB2  | 20       | 0.11          |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB3  | 20       | 0.11          |
| (1,370)  | 1:28:A:HIS:H     | 1:42:A:ASN:HA    | 14       | 0.11          |
| (1,370)  | 1:28:A:HIS:H     | 1:42:A:ASN:HA    | 16       | 0.11          |
| (1,317)  | 1:186:A:VAL:HG21 | 1:187:A:ASN:HB2  | 2        | 0.11          |
| (1,317)  | 1:186:A:VAL:HG21 | 1:187:A:ASN:HB3  | 2        | 0.11          |
| (1,317)  | 1:186:A:VAL:HG22 | 1:187:A:ASN:HB2  | 2        | 0.11          |
| (1,317)  | 1:186:A:VAL:HG22 | 1:187:A:ASN:HB3  | 2        | 0.11          |
| (1,317)  | 1:186:A:VAL:HG23 | 1:187:A:ASN:HB2  | 2        | 0.11          |
| (1,317)  | 1:186:A:VAL:HG23 | 1:187:A:ASN:HB3  | 2        | 0.11          |
| (1,39)   | 1:34:A:PHE:HD1   | 1:39:A:VAL:HB    | 11       | 0.11          |
| (1,39)   | 1:34:A:PHE:HD2   | 1:39:A:VAL:HB    | 11       | 0.11          |
| (3,2)    | 1:168:A:CYS:SG   | 2:302:A:ZN:ZN    | 19       | 0.1           |
| (2,9)    | 1:67:A:LEU:HD21  | 1:71:A:VAL:H     | 16       | 0.1           |
| (2,9)    | 1:67:A:LEU:HD22  | 1:71:A:VAL:H     | 16       | 0.1           |
| (2,9)    | 1:67:A:LEU:HD23  | 1:71:A:VAL:H     | 16       | 0.1           |
| (2,6)    | 1:32:A:GLY:H     | 1:40:A:PRO:HB2   | 7        | 0.1           |
| (1,6722) | 1:227:A:LYS:H    | 1:227:A:LYS:HG2  | 15       | 0.1           |
| (1,6722) | 1:227:A:LYS:H    | 1:227:A:LYS:HG3  | 15       | 0.1           |
| (1,6691) | 1:222:A:THR:HA   | 1:223:A:LEU:HD11 | 5        | 0.1           |
| (1,6691) | 1:222:A:THR:HA   | 1:223:A:LEU:HD12 | 5        | 0.1           |
| (1,6691) | 1:222:A:THR:HA   | 1:223:A:LEU:HD13 | 5        | 0.1           |
| (1,6691) | 1:222:A:THR:HA   | 1:223:A:LEU:HD21 | 5        | 0.1           |
| (1,6691) | 1:222:A:THR:HA   | 1:223:A:LEU:HD22 | 5        | 0.1           |
| (1,6691) | 1:222:A:THR:HA   | 1:223:A:LEU:HD23 | 5        | 0.1           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,5671) | 1:54:A:LEU:HD11  | 1:55:A:VAL:H    | 15       | 0.1           |
| (1,5671) | 1:54:A:LEU:HD12  | 1:55:A:VAL:H    | 15       | 0.1           |
| (1,5671) | 1:54:A:LEU:HD13  | 1:55:A:VAL:H    | 15       | 0.1           |
| (1,5671) | 1:54:A:LEU:HD21  | 1:55:A:VAL:H    | 15       | 0.1           |
| (1,5671) | 1:54:A:LEU:HD22  | 1:55:A:VAL:H    | 15       | 0.1           |
| (1,5671) | 1:54:A:LEU:HD23  | 1:55:A:VAL:H    | 15       | 0.1           |
| (1,5567) | 1:51:A:GLY:H     | 1:52:A:LEU:HD11 | 14       | 0.1           |
| (1,5567) | 1:51:A:GLY:H     | 1:52:A:LEU:HD12 | 14       | 0.1           |
| (1,5567) | 1:51:A:GLY:H     | 1:52:A:LEU:HD13 | 14       | 0.1           |
| (1,5567) | 1:51:A:GLY:H     | 1:52:A:LEU:HD21 | 14       | 0.1           |
| (1,5567) | 1:51:A:GLY:H     | 1:52:A:LEU:HD22 | 14       | 0.1           |
| (1,5567) | 1:51:A:GLY:H     | 1:52:A:LEU:HD23 | 14       | 0.1           |
| (1,5411) | 1:32:A:GLY:HA2   | 1:33:A:SER:H    | 9        | 0.1           |
| (1,5411) | 1:32:A:GLY:HA3   | 1:33:A:SER:H    | 9        | 0.1           |
| (1,5164) | 1:28:A:HIS:HE1   | 1:56:A:ASP:H    | 5        | 0.1           |
| (1,4675) | 1:208:A:PRO:HD3  | 1:210:A:HIS:H   | 19       | 0.1           |
| (1,4540) | 1:193:A:ILE:HA   | 1:197:A:LEU:H   | 12       | 0.1           |
| (1,4510) | 1:193:A:ILE:HG12 | 1:195:A:ASN:H   | 18       | 0.1           |
| (1,4155) | 1:158:A:LEU:H    | 1:161:A:TYR:HD1 | 15       | 0.1           |
| (1,4155) | 1:158:A:LEU:H    | 1:161:A:TYR:HD2 | 15       | 0.1           |
| (1,4040) | 1:148:A:GLY:H    | 1:151:A:GLU:H   | 9        | 0.1           |
| (1,4040) | 1:148:A:GLY:H    | 1:151:A:GLU:H   | 13       | 0.1           |
| (1,4040) | 1:148:A:GLY:H    | 1:151:A:GLU:H   | 15       | 0.1           |
| (1,3799) | 1:113:A:GLU:HB2  | 1:116:A:LYS:H   | 5        | 0.1           |
| (1,3799) | 1:113:A:GLU:HB3  | 1:116:A:LYS:H   | 5        | 0.1           |
| (1,3503) | 1:87:A:ALA:H     | 1:92:A:ILE:HD11 | 20       | 0.1           |
| (1,3503) | 1:87:A:ALA:H     | 1:92:A:ILE:HD12 | 20       | 0.1           |
| (1,3503) | 1:87:A:ALA:H     | 1:92:A:ILE:HD13 | 20       | 0.1           |
| (1,3410) | 1:77:A:LYS:HB2   | 1:79:A:VAL:H    | 16       | 0.1           |
| (1,3196) | 1:30:A:GLU:HA    | 1:59:A:TRP:HE1  | 2        | 0.1           |
| (1,3173) | 1:58:A:SER:H     | 1:95:A:ILE:H    | 20       | 0.1           |
| (1,3170) | 1:57:A:SER:H     | 1:84:A:ILE:HA   | 15       | 0.1           |
| (1,3100) | 1:48:A:THR:H     | 1:51:A:GLY:HA2  | 19       | 0.1           |
| (1,3058) | 1:46:A:LEU:H     | 1:54:A:LEU:HB3  | 7        | 0.1           |
| (1,2875) | 1:22:A:ASN:H     | 1:26:A:TRP:HE1  | 12       | 0.1           |
| (1,2618) | 1:57:A:SER:HA    | 1:91:A:ARG:HA   | 10       | 0.1           |
| (1,2509) | 1:148:A:GLY:H    | 1:192:A:SER:HB2 | 10       | 0.1           |
| (1,2394) | 1:114:A:LEU:HB2  | 1:150:A:THR:HB  | 18       | 0.1           |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD11 | 6        | 0.1           |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD12 | 6        | 0.1           |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD13 | 6        | 0.1           |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD11 | 8        | 0.1           |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD12  | 8        | 0.1           |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD13  | 8        | 0.1           |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD11  | 11       | 0.1           |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD12  | 11       | 0.1           |
| (1,2109) | 1:67:A:LEU:H     | 1:68:A:ILE:HD13  | 11       | 0.1           |
| (1,2097) | 1:58:A:SER:HB2   | 1:67:A:LEU:HG    | 2        | 0.1           |
| (1,2097) | 1:58:A:SER:HB2   | 1:67:A:LEU:HG    | 8        | 0.1           |
| (1,2097) | 1:58:A:SER:HB2   | 1:67:A:LEU:HG    | 15       | 0.1           |
| (1,2053) | 1:45:A:VAL:HA    | 1:53:A:VAL:HG21  | 7        | 0.1           |
| (1,2053) | 1:45:A:VAL:HA    | 1:53:A:VAL:HG22  | 7        | 0.1           |
| (1,2053) | 1:45:A:VAL:HA    | 1:53:A:VAL:HG23  | 7        | 0.1           |
| (1,1409) | 1:84:A:ILE:HG21  | 1:87:A:ALA:HA    | 17       | 0.1           |
| (1,1409) | 1:84:A:ILE:HG22  | 1:87:A:ALA:HA    | 17       | 0.1           |
| (1,1409) | 1:84:A:ILE:HG23  | 1:87:A:ALA:HA    | 17       | 0.1           |
| (1,1406) | 1:84:A:ILE:HG21  | 1:91:A:ARG:HA    | 20       | 0.1           |
| (1,1406) | 1:84:A:ILE:HG22  | 1:91:A:ARG:HA    | 20       | 0.1           |
| (1,1406) | 1:84:A:ILE:HG23  | 1:91:A:ARG:HA    | 20       | 0.1           |
| (1,899)  | 1:109:A:ALA:HB1  | 1:113:A:GLU:H    | 15       | 0.1           |
| (1,899)  | 1:109:A:ALA:HB2  | 1:113:A:GLU:H    | 15       | 0.1           |
| (1,899)  | 1:109:A:ALA:HB3  | 1:113:A:GLU:H    | 15       | 0.1           |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB1  | 16       | 0.1           |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB2  | 16       | 0.1           |
| (1,867)  | 1:57:A:SER:H     | 1:105:A:ALA:HB3  | 16       | 0.1           |
| (1,822)  | 1:95:A:ILE:HG12  | 1:99:A:LYS:HA    | 18       | 0.1           |
| (1,786)  | 1:95:A:ILE:HD11  | 1:122:A:GLU:HA   | 18       | 0.1           |
| (1,786)  | 1:95:A:ILE:HD12  | 1:122:A:GLU:HA   | 18       | 0.1           |
| (1,786)  | 1:95:A:ILE:HD13  | 1:122:A:GLU:HA   | 18       | 0.1           |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD11 | 12       | 0.1           |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD12 | 12       | 0.1           |
| (1,329)  | 1:222:A:THR:HG21 | 1:226:A:LEU:HD13 | 12       | 0.1           |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD11 | 12       | 0.1           |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD12 | 12       | 0.1           |
| (1,329)  | 1:222:A:THR:HG22 | 1:226:A:LEU:HD13 | 12       | 0.1           |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD11 | 12       | 0.1           |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD12 | 12       | 0.1           |
| (1,329)  | 1:222:A:THR:HG23 | 1:226:A:LEU:HD13 | 12       | 0.1           |
| (1,317)  | 1:186:A:VAL:HG21 | 1:187:A:ASN:HB2  | 8        | 0.1           |
| (1,317)  | 1:186:A:VAL:HG21 | 1:187:A:ASN:HB3  | 8        | 0.1           |
| (1,317)  | 1:186:A:VAL:HG22 | 1:187:A:ASN:HB2  | 8        | 0.1           |
| (1,317)  | 1:186:A:VAL:HG22 | 1:187:A:ASN:HB3  | 8        | 0.1           |
| (1,317)  | 1:186:A:VAL:HG23 | 1:187:A:ASN:HB2  | 8        | 0.1           |
| (1,317)  | 1:186:A:VAL:HG23 | 1:187:A:ASN:HB3  | 8        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found