



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 10:16 PM UTC

PDB ID : 7DTH / pdb\_00007dth  
BMRB ID : 36405  
Title : Solution structure of RPB6, common subunit of RNA polymerases I, II, and III  
Authors : Okuda, M.; Nishimura, Y.  
Deposited on : 2021-01-05

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

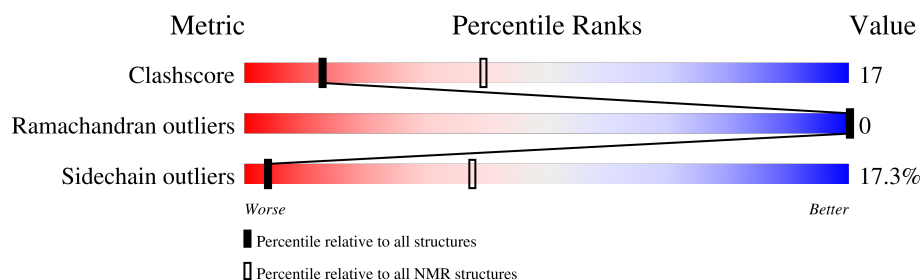
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 91%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 130    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:35-A:41, A:52-A:126 (82) | 0.48              | 17           |

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1981 atoms, of which 968 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 127      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1981  | 625 | 968 | 166 | 216 | 6 |       |

There are 3 discrepancies between the modelled and reference sequences:

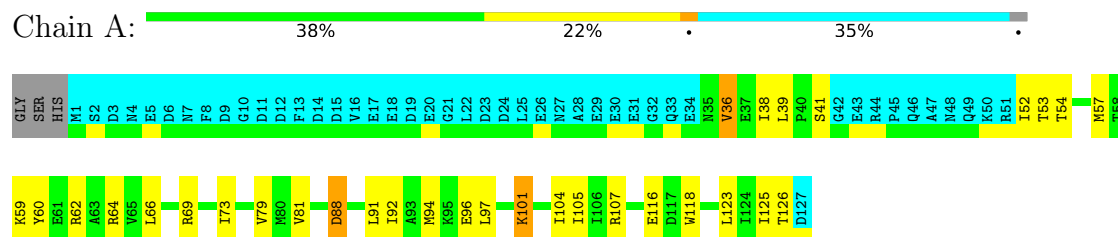
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -2      | GLY      | -      | expression tag | UNP P61218 |
| A     | -1      | SER      | -      | expression tag | UNP P61218 |
| A     | 0       | HIS      | -      | expression tag | UNP P61218 |

## 4 Residue-property plots

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

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

- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2

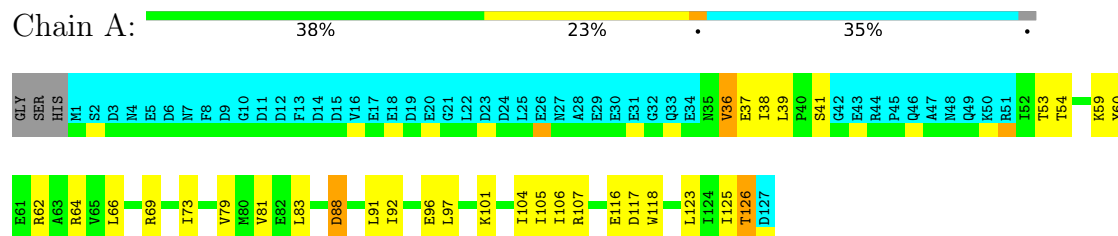


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

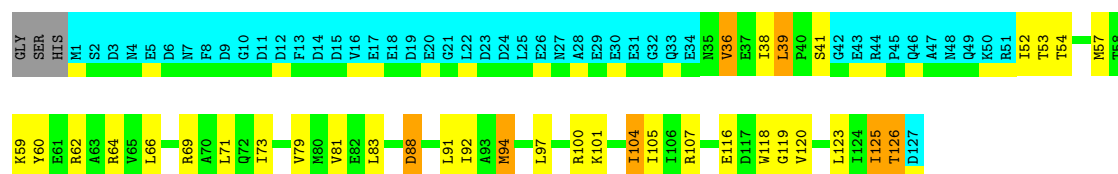
- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2



#### 4.2.2 Score per residue for model 2

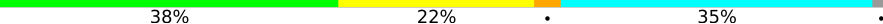
- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2

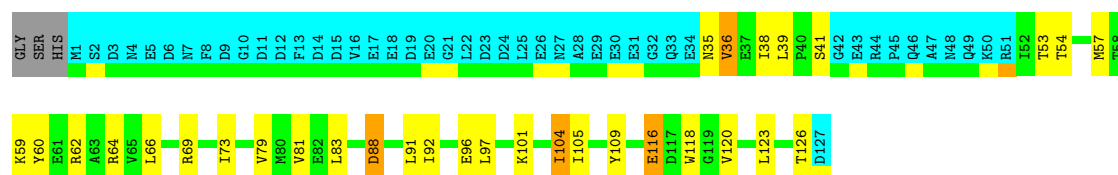




### 4.2.3 Score per residue for model 3

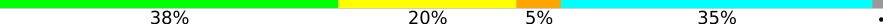
- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2

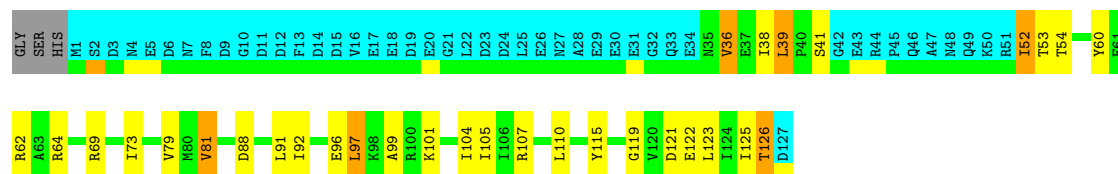
Chain A: 



### 4.2.4 Score per residue for model 4

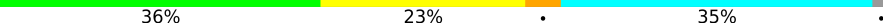
- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2

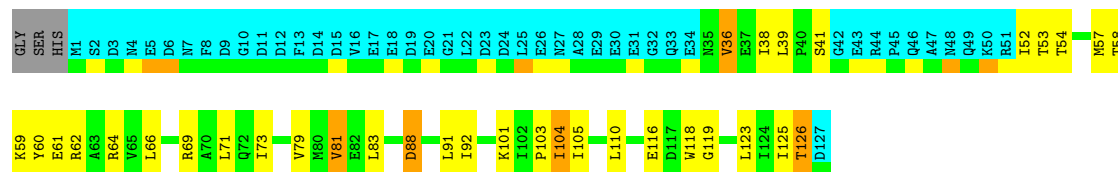
Chain A: 



### 4.2.5 Score per residue for model 5

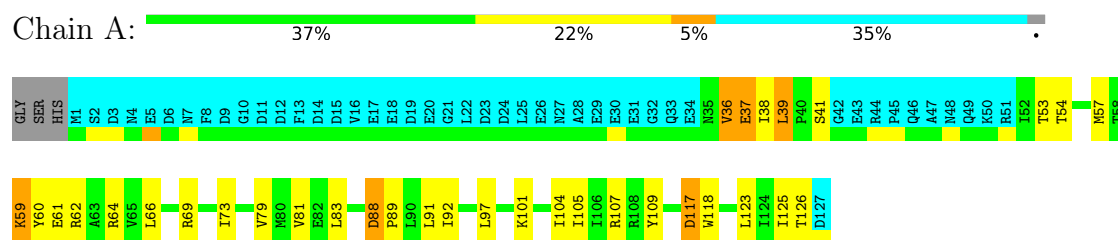
- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain A: 



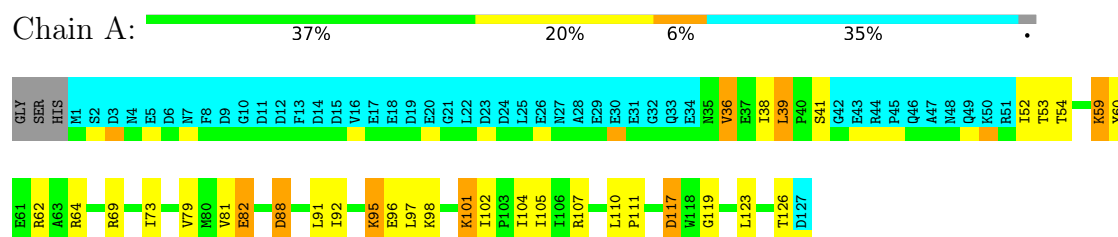
### 4.2.6 Score per residue for model 6

- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2



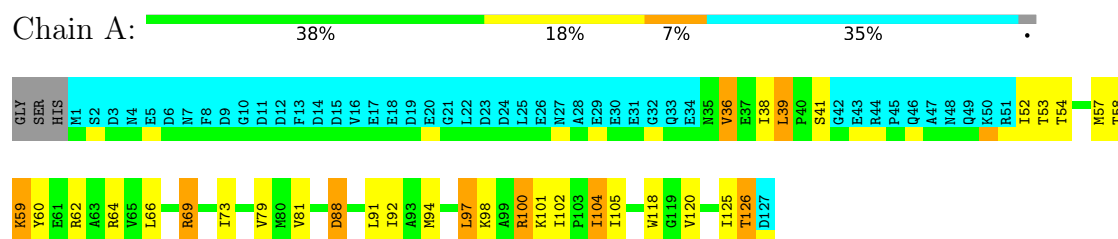
#### 4.2.7 Score per residue for model 7

- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2



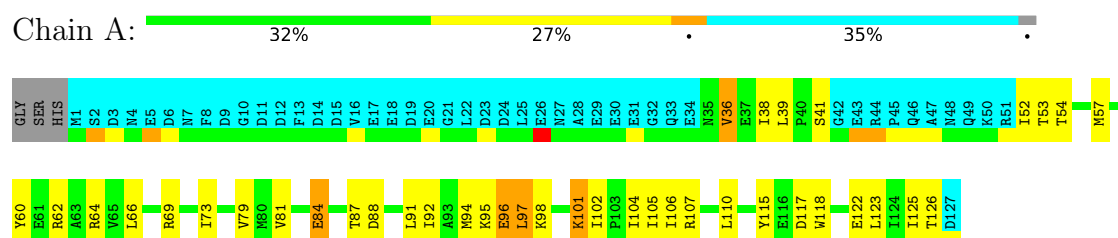
#### 4.2.8 Score per residue for model 8

- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2



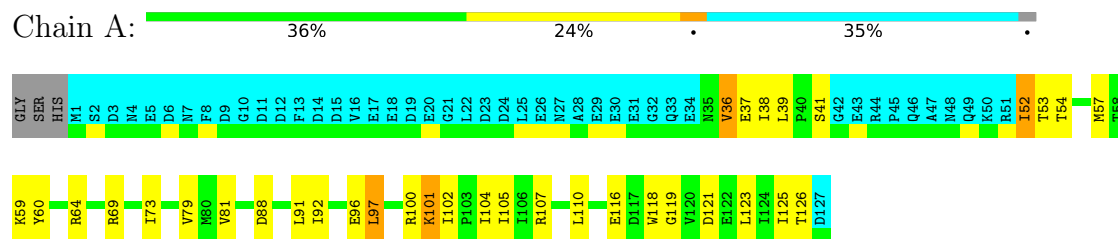
#### 4.2.9 Score per residue for model 9

- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2



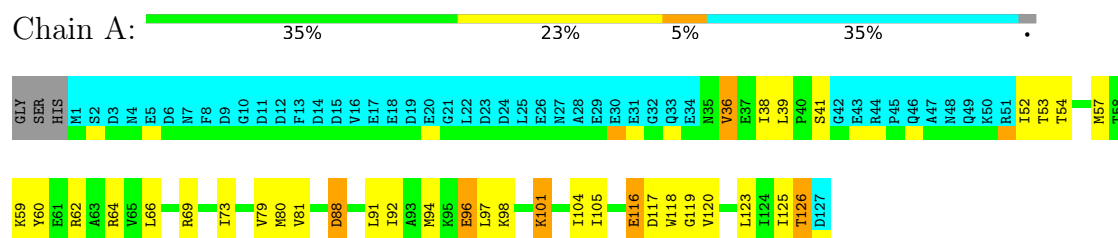
### 4.2.10 Score per residue for model 10

- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2



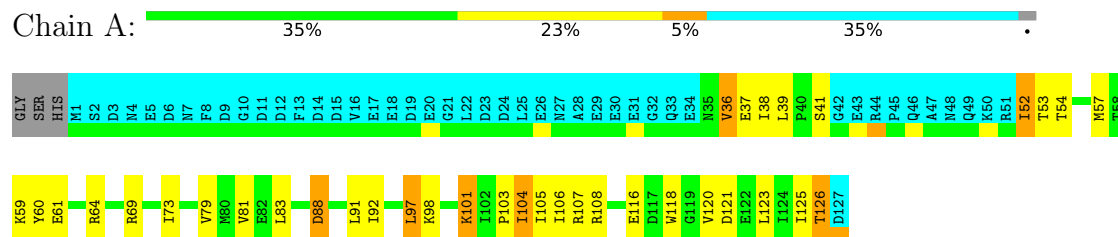
### 4.2.11 Score per residue for model 11

- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2



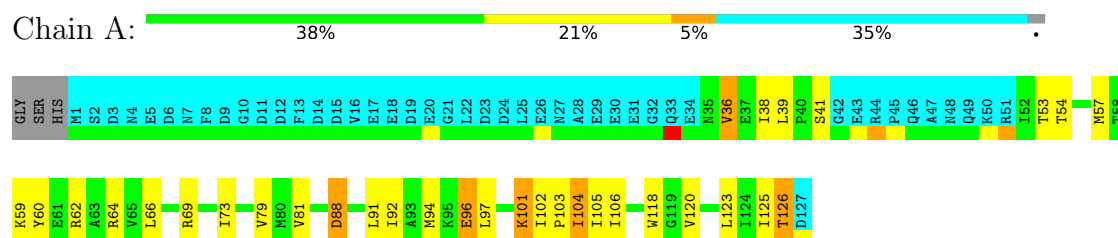
### 4.2.12 Score per residue for model 12

- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2



### 4.2.13 Score per residue for model 13

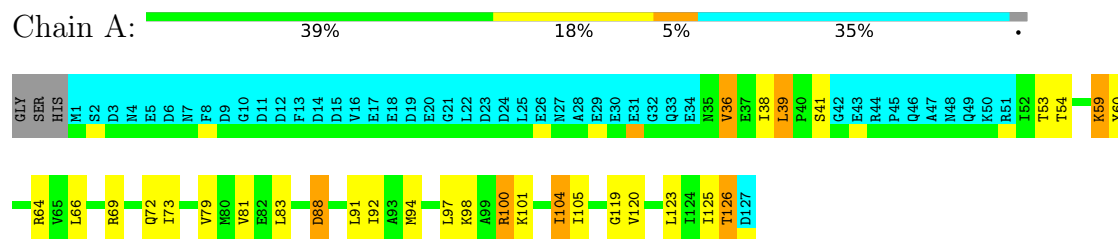
- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2





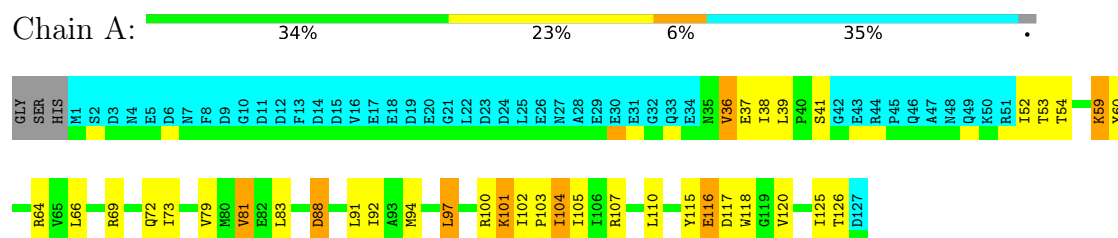
#### 4.2.14 Score per residue for model 14

- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2



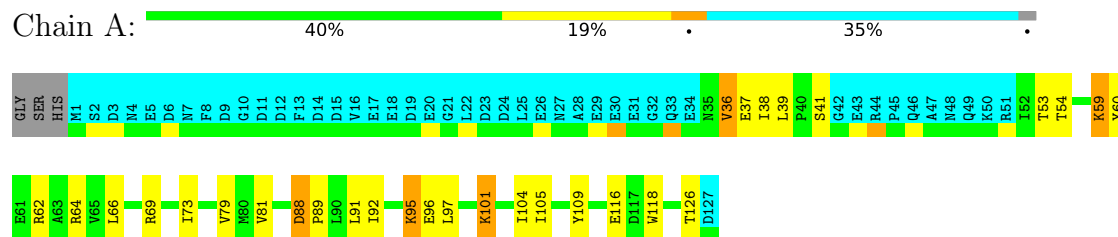
#### 4.2.15 Score per residue for model 15

- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2



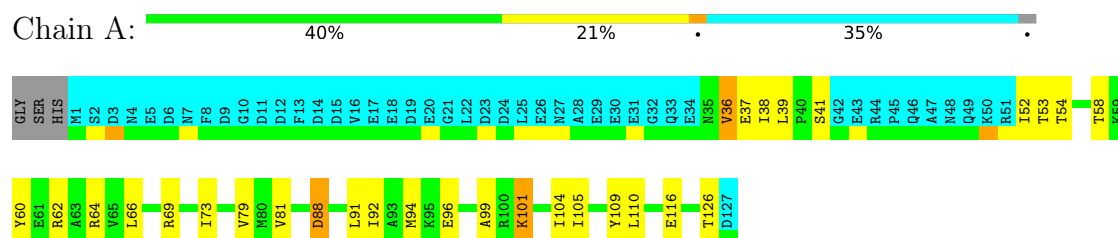
#### 4.2.16 Score per residue for model 16

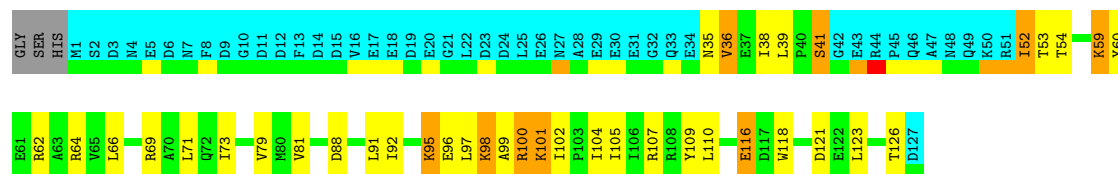
- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2



#### 4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: DNA-directed RNA polymerases I, II, and III subunit RPABC2





## 5 Refinement protocol and experimental data overview

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

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 |
|---------------|-----------------------|---------|
| X-PLOR NIH    | structure calculation |         |
| X-PLOR NIH    | refinement            |         |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| Chemical shift file(s)                       | working_cs.cif |
|----------------------------------------------|----------------|
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1512           |
| Number of shifts mapped to atoms             | 1512           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 91%            |

## 6 Model quality

### 6.1 Standard geometry

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     | 652   | 685      | 685      | 22±3    |
| All | All   | 13040 | 13700    | 13700    | 442     |

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 17.

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

| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:88:ASP:HB3  | 1:A:91:LEU:HD12  | 0.95     | 1.38        | 8      | 20    |
| 1:A:41:SER:HB3  | 1:A:105:ILE:HG13 | 0.84     | 1.48        | 20     | 15    |
| 1:A:81:VAL:HG11 | 1:A:96:GLU:HA    | 0.84     | 1.47        | 17     | 10    |
| 1:A:41:SER:HA   | 1:A:105:ILE:HG12 | 0.79     | 1.52        | 4      | 5     |
| 1:A:36:VAL:HG13 | 1:A:60:TYR:HE2   | 0.78     | 1.37        | 11     | 6     |
| 1:A:66:LEU:HD13 | 1:A:94:MET:HG2   | 0.77     | 1.55        | 14     | 10    |
| 1:A:81:VAL:HG12 | 1:A:101:LYS:HD3  | 0.76     | 1.56        | 18     | 9     |
| 1:A:81:VAL:HG21 | 1:A:95:LYS:HB3   | 0.75     | 1.59        | 20     | 4     |
| 1:A:57:MET:HE1  | 1:A:106:ILE:HD11 | 0.70     | 1.62        | 19     | 1     |
| 1:A:36:VAL:HG13 | 1:A:60:TYR:HE1   | 0.69     | 1.47        | 14     | 8     |
| 1:A:118:TRP:HB3 | 1:A:123:LEU:HD11 | 0.68     | 1.65        | 6      | 9     |
| 1:A:36:VAL:HG22 | 1:A:60:TYR:HE2   | 0.66     | 1.50        | 20     | 2     |
| 1:A:36:VAL:HG22 | 1:A:60:TYR:HE1   | 0.66     | 1.51        | 1      | 2     |
| 1:A:81:VAL:HG13 | 1:A:96:GLU:HG3   | 0.63     | 1.69        | 9      | 4     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:79:VAL:HG12 | 1:A:81:VAL:H     | 0.63     | 1.53        | 3      | 19    |
| 1:A:52:ILE:HD13 | 1:A:110:LEU:HD21 | 0.62     | 1.71        | 7      | 5     |
| 1:A:52:ILE:HD11 | 1:A:116:GLU:HB2  | 0.62     | 1.69        | 12     | 2     |
| 1:A:36:VAL:HG13 | 1:A:60:TYR:CE1   | 0.62     | 2.30        | 7      | 10    |
| 1:A:38:ILE:HD11 | 1:A:64:ARG:HB3   | 0.62     | 1.69        | 6      | 16    |
| 1:A:36:VAL:HG13 | 1:A:60:TYR:CE2   | 0.62     | 2.29        | 17     | 10    |
| 1:A:57:MET:HB3  | 1:A:125:ILE:HD12 | 0.62     | 1.71        | 18     | 4     |
| 1:A:99:ALA:HB1  | 1:A:101:LYS:HD2  | 0.60     | 1.72        | 20     | 2     |
| 1:A:39:LEU:HD11 | 1:A:107:ARG:HB2  | 0.60     | 1.72        | 6      | 2     |
| 1:A:69:ARG:O    | 1:A:73:ILE:HD12  | 0.59     | 1.97        | 20     | 20    |
| 1:A:57:MET:HE1  | 1:A:120:VAL:HG22 | 0.59     | 1.75        | 11     | 5     |
| 1:A:98:LYS:HE3  | 1:A:98:LYS:HA    | 0.59     | 1.75        | 18     | 1     |
| 1:A:59:LYS:HD3  | 1:A:59:LYS:C     | 0.58     | 2.22        | 12     | 1     |
| 1:A:60:TYR:O    | 1:A:64:ARG:HG2   | 0.56     | 2.00        | 18     | 2     |
| 1:A:57:MET:CB   | 1:A:125:ILE:HD12 | 0.56     | 2.30        | 2      | 5     |
| 1:A:41:SER:HA   | 1:A:105:ILE:CG1  | 0.56     | 2.27        | 4      | 2     |
| 1:A:81:VAL:HG13 | 1:A:96:GLU:HG2   | 0.56     | 1.77        | 10     | 3     |
| 1:A:59:LYS:HD2  | 1:A:59:LYS:C     | 0.56     | 2.25        | 14     | 7     |
| 1:A:52:ILE:HD11 | 1:A:110:LEU:HD21 | 0.54     | 1.79        | 4      | 3     |
| 1:A:52:ILE:HG13 | 1:A:116:GLU:OE2  | 0.54     | 2.02        | 11     | 1     |
| 1:A:37:GLU:HB2  | 1:A:109:TYR:HE1  | 0.53     | 1.63        | 6      | 2     |
| 1:A:97:LEU:HD12 | 1:A:97:LEU:O     | 0.53     | 2.04        | 14     | 14    |
| 1:A:98:LYS:HA   | 1:A:100:ARG:NH2  | 0.53     | 2.18        | 8      | 3     |
| 1:A:107:ARG:HD2 | 1:A:115:TYR:CD1  | 0.53     | 2.38        | 15     | 1     |
| 1:A:81:VAL:CG1  | 1:A:96:GLU:HG3   | 0.53     | 2.34        | 9      | 3     |
| 1:A:61:GLU:HG2  | 1:A:106:ILE:HG21 | 0.53     | 1.78        | 12     | 1     |
| 1:A:41:SER:CA   | 1:A:105:ILE:HG12 | 0.53     | 2.34        | 10     | 5     |
| 1:A:88:ASP:CB   | 1:A:91:LEU:HD12  | 0.53     | 2.26        | 18     | 1     |
| 1:A:36:VAL:HG22 | 1:A:60:TYR:CE1   | 0.52     | 2.39        | 5      | 3     |
| 1:A:81:VAL:CG1  | 1:A:96:GLU:HA    | 0.52     | 2.28        | 17     | 7     |
| 1:A:66:LEU:CD1  | 1:A:94:MET:HG2   | 0.52     | 2.35        | 11     | 7     |
| 1:A:38:ILE:CD1  | 1:A:64:ARG:HB3   | 0.52     | 2.34        | 6      | 1     |
| 1:A:57:MET:HE1  | 1:A:106:ILE:CD1  | 0.52     | 2.34        | 19     | 3     |
| 1:A:99:ALA:CB   | 1:A:101:LYS:HD2  | 0.51     | 2.35        | 4      | 2     |
| 1:A:62:ARG:HG3  | 1:A:97:LEU:CD2   | 0.51     | 2.35        | 20     | 2     |
| 1:A:57:MET:HG3  | 1:A:61:GLU:HB3   | 0.51     | 1.81        | 6      | 1     |
| 1:A:62:ARG:O    | 1:A:66:LEU:HG    | 0.51     | 2.06        | 17     | 10    |
| 1:A:91:LEU:HA   | 1:A:94:MET:HE2   | 0.51     | 1.81        | 17     | 1     |
| 1:A:73:ILE:HB   | 1:A:89:PRO:HB3   | 0.50     | 1.83        | 6      | 2     |
| 1:A:69:ARG:HA   | 1:A:72:GLN:HG2   | 0.50     | 1.83        | 15     | 1     |
| 1:A:62:ARG:HG3  | 1:A:97:LEU:HD21  | 0.50     | 1.83        | 20     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:57:MET:SD    | 1:A:61:GLU:HB3   | 0.50     | 2.47        | 12     | 1     |
| 1:A:36:VAL:HG22  | 1:A:60:TYR:CE2   | 0.50     | 2.37        | 20     | 1     |
| 1:A:39:LEU:HD12  | 1:A:105:ILE:HG22 | 0.49     | 1.85        | 14     | 2     |
| 1:A:79:VAL:CG2   | 1:A:92:ILE:HG21  | 0.49     | 2.37        | 7      | 20    |
| 1:A:38:ILE:HD11  | 1:A:64:ARG:CB    | 0.49     | 2.37        | 2      | 12    |
| 1:A:88:ASP:HB3   | 1:A:91:LEU:CD1   | 0.48     | 2.28        | 18     | 3     |
| 1:A:101:LYS:O    | 1:A:103:PRO:HD3  | 0.48     | 2.08        | 15     | 3     |
| 1:A:108:ARG:HD3  | 1:A:118:TRP:CD1  | 0.48     | 2.42        | 12     | 1     |
| 1:A:107:ARG:HD3  | 1:A:117:ASP:OD1  | 0.47     | 2.09        | 15     | 1     |
| 1:A:41:SER:HA    | 1:A:105:ILE:HD12 | 0.47     | 1.85        | 2      | 3     |
| 1:A:82:GLU:H     | 1:A:82:GLU:CD    | 0.47     | 2.18        | 7      | 1     |
| 1:A:106:ILE:O    | 1:A:118:TRP:HB2  | 0.47     | 2.10        | 13     | 3     |
| 1:A:36:VAL:HG21  | 1:A:106:ILE:HG23 | 0.46     | 1.86        | 1      | 1     |
| 1:A:84:GLU:CD    | 1:A:95:LYS:HZ1   | 0.46     | 2.17        | 9      | 1     |
| 1:A:107:ARG:HA   | 1:A:116:GLU:O    | 0.46     | 2.10        | 15     | 1     |
| 1:A:37:GLU:OE1   | 1:A:107:ARG:HD2  | 0.46     | 2.10        | 18     | 2     |
| 1:A:79:VAL:HG21  | 1:A:92:ILE:HD13  | 0.46     | 1.86        | 9      | 7     |
| 1:A:97:LEU:HD11  | 1:A:125:ILE:HG21 | 0.46     | 1.87        | 4      | 2     |
| 1:A:79:VAL:HG22  | 1:A:92:ILE:HG21  | 0.46     | 1.87        | 7      | 2     |
| 1:A:58:THR:O     | 1:A:62:ARG:HB2   | 0.46     | 2.11        | 8      | 1     |
| 1:A:37:GLU:HB2   | 1:A:109:TYR:HE2  | 0.46     | 1.71        | 16     | 1     |
| 1:A:107:ARG:HD2  | 1:A:115:TYR:CD2  | 0.46     | 2.45        | 4      | 2     |
| 1:A:35:ASN:ND2   | 1:A:109:TYR:HB2  | 0.46     | 2.26        | 20     | 1     |
| 1:A:37:GLU:HB2   | 1:A:107:ARG:HB3  | 0.45     | 1.86        | 1      | 4     |
| 1:A:36:VAL:CG1   | 1:A:60:TYR:HE1   | 0.45     | 2.24        | 7      | 3     |
| 1:A:61:GLU:OE1   | 1:A:108:ARG:HD2  | 0.45     | 2.11        | 12     | 1     |
| 1:A:104:ILE:O    | 1:A:120:VAL:HG23 | 0.45     | 2.10        | 14     | 7     |
| 1:A:41:SER:CB    | 1:A:105:ILE:HG13 | 0.45     | 2.41        | 19     | 1     |
| 1:A:69:ARG:HA    | 1:A:72:GLN:HG3   | 0.45     | 1.86        | 14     | 1     |
| 1:A:125:ILE:HG22 | 1:A:126:THR:N    | 0.45     | 2.27        | 12     | 9     |
| 1:A:81:VAL:HG22  | 1:A:96:GLU:HG3   | 0.44     | 1.89        | 1      | 3     |
| 1:A:119:GLY:O    | 1:A:123:LEU:HD13 | 0.44     | 2.13        | 18     | 9     |
| 1:A:39:LEU:HD11  | 1:A:107:ARG:HD3  | 0.44     | 1.88        | 7      | 1     |
| 1:A:37:GLU:HB2   | 1:A:109:TYR:CE1  | 0.44     | 2.47        | 6      | 1     |
| 1:A:98:LYS:HA    | 1:A:100:ARG:HH21 | 0.43     | 1.73        | 8      | 2     |
| 1:A:38:ILE:HD11  | 1:A:64:ARG:HB2   | 0.43     | 1.88        | 9      | 2     |
| 1:A:97:LEU:HD11  | 1:A:125:ILE:HG13 | 0.43     | 1.90        | 2      | 1     |
| 1:A:57:MET:HG3   | 1:A:61:GLU:HB2   | 0.43     | 1.89        | 5      | 1     |
| 1:A:36:VAL:CG1   | 1:A:60:TYR:HE2   | 0.43     | 2.19        | 11     | 2     |
| 1:A:59:LYS:HB2   | 1:A:62:ARG:NH2   | 0.43     | 2.28        | 16     | 1     |
| 1:A:35:ASN:HA    | 1:A:60:TYR:OH    | 0.43     | 2.14        | 3      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:39:LEU:HB2   | 1:A:105:ILE:HB   | 0.43     | 1.89        | 4      | 1     |
| 1:A:110:LEU:HD22 | 1:A:111:PRO:HD2  | 0.43     | 1.91        | 7      | 1     |
| 1:A:99:ALA:O     | 1:A:101:LYS:HD2  | 0.43     | 2.14        | 17     | 1     |
| 1:A:52:ILE:HG12  | 1:A:110:LEU:HD11 | 0.43     | 1.91        | 10     | 1     |
| 1:A:38:ILE:CG1   | 1:A:64:ARG:HB3   | 0.42     | 2.44        | 6      | 2     |
| 1:A:100:ARG:CZ   | 1:A:125:ILE:HG12 | 0.42     | 2.44        | 2      | 1     |
| 1:A:52:ILE:HG13  | 1:A:116:GLU:OE1  | 0.42     | 2.15        | 5      | 1     |
| 1:A:59:LYS:HD2   | 1:A:60:TYR:N     | 0.42     | 2.30        | 15     | 1     |
| 1:A:59:LYS:HD2   | 1:A:59:LYS:O     | 0.42     | 2.15        | 3      | 1     |
| 1:A:103:PRO:O    | 1:A:104:ILE:HG13 | 0.42     | 2.15        | 13     | 2     |
| 1:A:97:LEU:O     | 1:A:97:LEU:HD12  | 0.42     | 2.15        | 7      | 1     |
| 1:A:97:LEU:HD12  | 1:A:97:LEU:C     | 0.42     | 2.40        | 8      | 3     |
| 1:A:118:TRP:HB3  | 1:A:123:LEU:CD1  | 0.42     | 2.41        | 6      | 1     |
| 1:A:81:VAL:CG1   | 1:A:101:LYS:HD3  | 0.42     | 2.44        | 11     | 2     |
| 1:A:125:ILE:HD13 | 1:A:125:ILE:N    | 0.41     | 2.31        | 2      | 1     |
| 1:A:52:ILE:HD13  | 1:A:110:LEU:HD11 | 0.41     | 1.93        | 18     | 1     |
| 1:A:100:ARG:HH11 | 1:A:125:ILE:HG12 | 0.41     | 1.76        | 18     | 1     |
| 1:A:58:THR:O     | 1:A:62:ARG:HB3   | 0.40     | 2.16        | 17     | 1     |
| 1:A:81:VAL:CG1   | 1:A:96:GLU:HG2   | 0.40     | 2.46        | 18     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured     | Allowed    | Outliers   | Percentiles |     |
|-----|-------|-----------------|--------------|------------|------------|-------------|-----|
| 1   | A     | 82/130 (63%)    | 76±1 (92±1%) | 6±1 (8±1%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 1640/2600 (63%) | 1514 (92%)   | 126 (8%)   | 0 (0%)     | 100         | 100 |

There are no Ramachandran outliers.

### 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     | 72/113 (64%)    | 60±2 (83±3%) | 12±2 (17±3%) | 4           | 38 |
| All | All   | 1440/2260 (64%) | 1191 (83%)   | 249 (17%)    | 4           | 38 |

All 34 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     | 36  | VAL  | 20             |
| 1   | A     | 39  | LEU  | 20             |
| 1   | A     | 53  | THR  | 20             |
| 1   | A     | 54  | THR  | 20             |
| 1   | A     | 104 | ILE  | 20             |
| 1   | A     | 126 | THR  | 20             |
| 1   | A     | 101 | LYS  | 19             |
| 1   | A     | 88  | ASP  | 15             |
| 1   | A     | 59  | LYS  | 13             |
| 1   | A     | 102 | ILE  | 9              |
| 1   | A     | 83  | LEU  | 8              |
| 1   | A     | 52  | ILE  | 6              |
| 1   | A     | 97  | LEU  | 6              |
| 1   | A     | 121 | ASP  | 6              |
| 1   | A     | 116 | GLU  | 5              |
| 1   | A     | 100 | ARG  | 5              |
| 1   | A     | 81  | VAL  | 4              |
| 1   | A     | 95  | LYS  | 4              |
| 1   | A     | 98  | LYS  | 4              |
| 1   | A     | 117 | ASP  | 3              |
| 1   | A     | 71  | LEU  | 3              |
| 1   | A     | 58  | THR  | 3              |
| 1   | A     | 96  | GLU  | 3              |
| 1   | A     | 69  | ARG  | 2              |
| 1   | A     | 84  | GLU  | 2              |
| 1   | A     | 94  | MET  | 1              |
| 1   | A     | 125 | ILE  | 1              |
| 1   | A     | 122 | GLU  | 1              |
| 1   | A     | 37  | GLU  | 1              |
| 1   | A     | 82  | GLU  | 1              |
| 1   | A     | 87  | THR  | 1              |
| 1   | A     | 80  | MET  | 1              |
| 1   | A     | 41  | SER  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 107 | ARG  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 88% 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                  | 1512 |
| Number of shifts mapped to atoms        | 1512 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 2    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 127      | $-0.04 \pm 0.11$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 119      | $0.08 \pm 0.10$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 127      | $-0.03 \pm 0.13$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 120      | $-1.69 \pm 0.23$                | Should be applied          |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1071 atoms were assigned a chemical shift out of a possible 1174. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 402/402 (100%) | 162/162 (100%) | 164/164 (100%)  | 76/76 (100%)    |
| Sidechain | 641/724 (89%)  | 429/476 (90%)  | 204/224 (91%)   | 8/24 (33%)      |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 28/48 (58%)     | 14/22 (64%)          | 13/25 (52%)           | 1/1 (100%)            |
| Overall  | 1071/1174 (91%) | 605/660 (92%)        | 381/413 (92%)         | 85/101 (84%)          |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 1512 atoms were assigned a chemical shift out of a possible 1714. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 625/629 (99%)   | 251/255 (98%)        | 254/254 (100%)        | 120/120 (100%)        |
| Sidechain | 847/1017 (83%)  | 557/652 (85%)        | 275/327 (84%)         | 15/38 (39%)           |
| Aromatic  | 40/68 (59%)     | 20/32 (62%)          | 19/35 (54%)           | 1/1 (100%)            |
| Overall   | 1512/1714 (88%) | 828/939 (88%)        | 548/616 (89%)         | 136/159 (86%)         |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

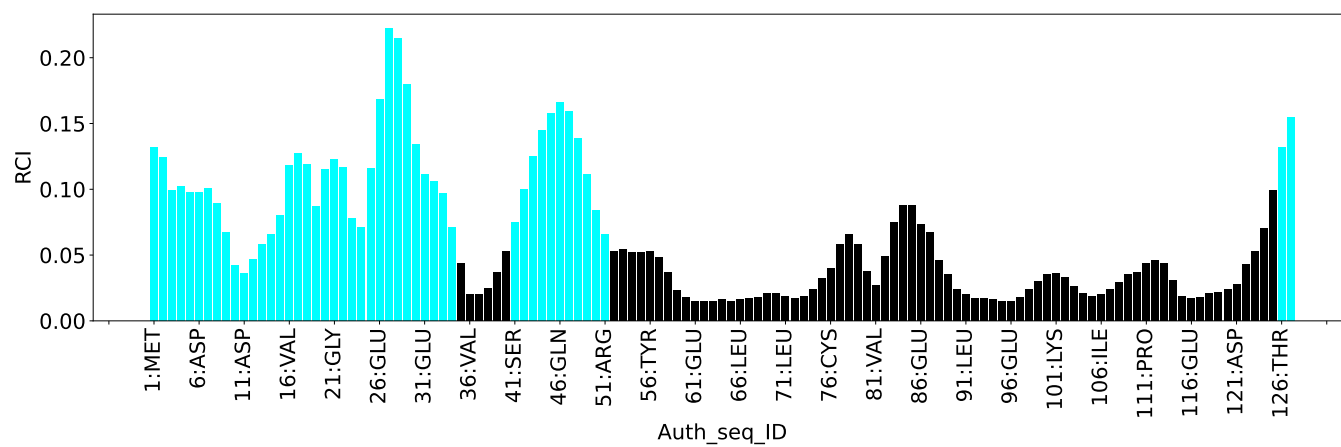
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 69  | ARG  | HE   | 11.37      | 4.52 – 10.19        | 7.1     |
| 1       | A     | 51  | ARG  | HD3  | 1.35       | 1.81 – 4.39         | -6.8    |

#### 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:



## 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                                | 1853  |
| Intra-residue ( $ i-j =0$ )                              | 279   |
| Sequential ( $ i-j =1$ )                                 | 521   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 361   |
| Long range ( $ i-j \geq 5$ )                             | 622   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 70    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 273   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 16.4  |
| Number of long range restraints per residue <sup>1</sup> | 5.0   |

<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)  | 15.2                                   | 0.2     |
| 0.2-0.5 (Medium) | 11.7                                   | 0.5     |
| >0.5 (Large)     | 1.4                                    | 0.64    |

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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 9.5                                    | 4.74    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

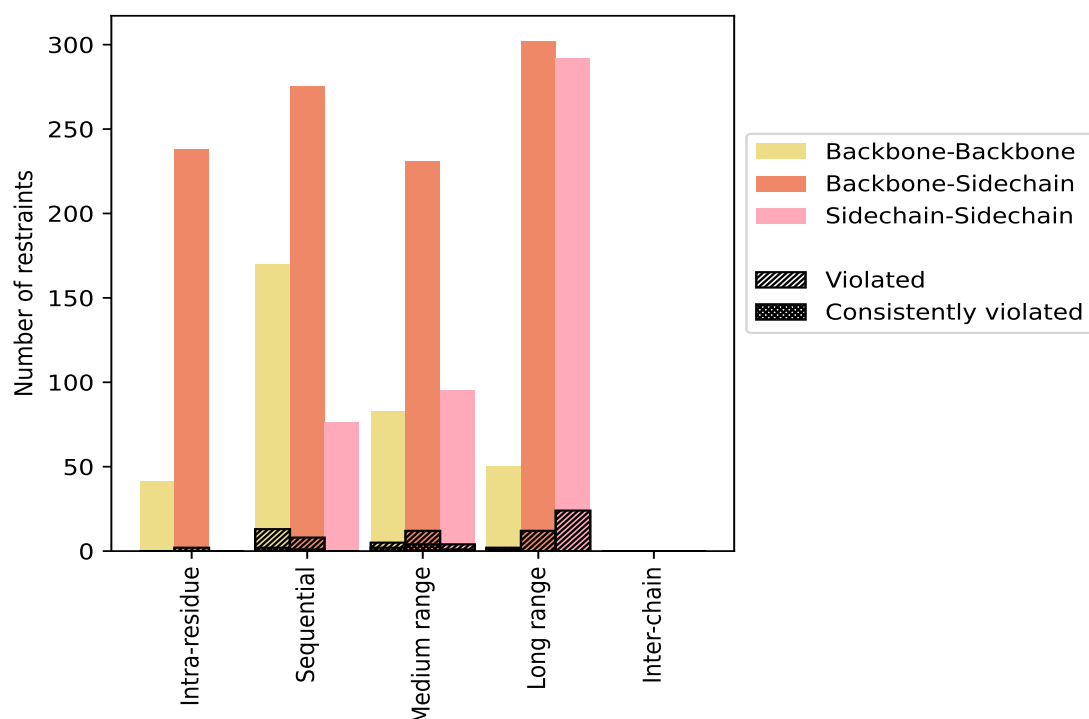
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>279</b>  | <b>15.1</b>    | <b>2</b>              | <b>0.7</b>     | <b>0.1</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 41          | 2.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 238         | 12.8           | 2                     | 0.8            | 0.1            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>521</b>  | <b>28.1</b>    | <b>21</b>             | <b>4.0</b>     | <b>1.1</b>     | <b>3</b>                           | <b>0.6</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 170         | 9.2            | 13                    | 7.6            | 0.7            | 2                                  | 1.2            | 0.1            |
| Backbone-Sidechain                                                          | 275         | 14.8           | 8                     | 2.9            | 0.4            | 1                                  | 0.4            | 0.1            |
| Sidechain-Sidechain                                                         | 76          | 4.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>361</b>  | <b>19.5</b>    | <b>19</b>             | <b>5.3</b>     | <b>1.0</b>     | <b>7</b>                           | <b>1.9</b>     | <b>0.4</b>     |
| Backbone-Backbone                                                           | 83          | 4.5            | 5                     | 6.0            | 0.3            | 2                                  | 2.4            | 0.1            |
| Backbone-Sidechain                                                          | 183         | 9.9            | 10                    | 5.5            | 0.5            | 4                                  | 2.2            | 0.2            |
| Sidechain-Sidechain                                                         | 95          | 5.1            | 4                     | 4.2            | 0.2            | 1                                  | 1.1            | 0.1            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>622</b>  | <b>33.6</b>    | <b>38</b>             | <b>6.1</b>     | <b>2.1</b>     | <b>1</b>                           | <b>0.2</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 50          | 2.7            | 2                     | 4.0            | 0.1            | 1                                  | 2.0            | 0.1            |
| Backbone-Sidechain                                                          | 280         | 15.1           | 12                    | 4.3            | 0.6            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 292         | 15.8           | 24                    | 8.2            | 1.3            | 0                                  | 0.0            | 0.0            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>70</b>   | <b>3.8</b>     | <b>2</b>              | <b>2.9</b>     | <b>0.1</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>1853</b> | <b>100.0</b>   | <b>82</b>             | <b>4.4</b>     | <b>4.4</b>     | <b>11</b>                          | <b>0.6</b>     | <b>0.6</b>     |
| Backbone-Backbone                                                           | 344         | 18.6           | 20                    | 5.8            | 1.1            | 5                                  | 1.5            | 0.3            |
| Backbone-Sidechain                                                          | 1046        | 56.4           | 34                    | 3.3            | 1.8            | 5                                  | 0.5            | 0.3            |
| Sidechain-Sidechain                                                         | 463         | 25.0           | 28                    | 6.0            | 1.5            | 1                                  | 0.2            | 0.1            |

<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                    | 7               | 11              | 7               | 0               | 25    | 0.24     | 0.58    | 0.14                | 0.15       |
| 2        | 1                    | 7               | 12              | 11              | 0               | 31    | 0.22     | 0.6     | 0.13                | 0.18       |
| 3        | 0                    | 10              | 11              | 9               | 0               | 30    | 0.23     | 0.61    | 0.13                | 0.18       |
| 4        | 1                    | 6               | 13              | 9               | 0               | 29    | 0.22     | 0.61    | 0.13                | 0.16       |
| 5        | 1                    | 4               | 10              | 7               | 0               | 22    | 0.24     | 0.56    | 0.12                | 0.22       |
| 6        | 1                    | 9               | 15              | 9               | 0               | 34    | 0.22     | 0.6     | 0.12                | 0.16       |
| 7        | 1                    | 10              | 12              | 9               | 0               | 32    | 0.22     | 0.59    | 0.11                | 0.19       |
| 8        | 0                    | 7               | 11              | 10              | 0               | 28    | 0.24     | 0.63    | 0.14                | 0.2        |
| 9        | 1                    | 6               | 10              | 9               | 0               | 26    | 0.25     | 0.61    | 0.13                | 0.19       |
| 10       | 2                    | 9               | 12              | 7               | 0               | 30    | 0.24     | 0.57    | 0.12                | 0.2        |

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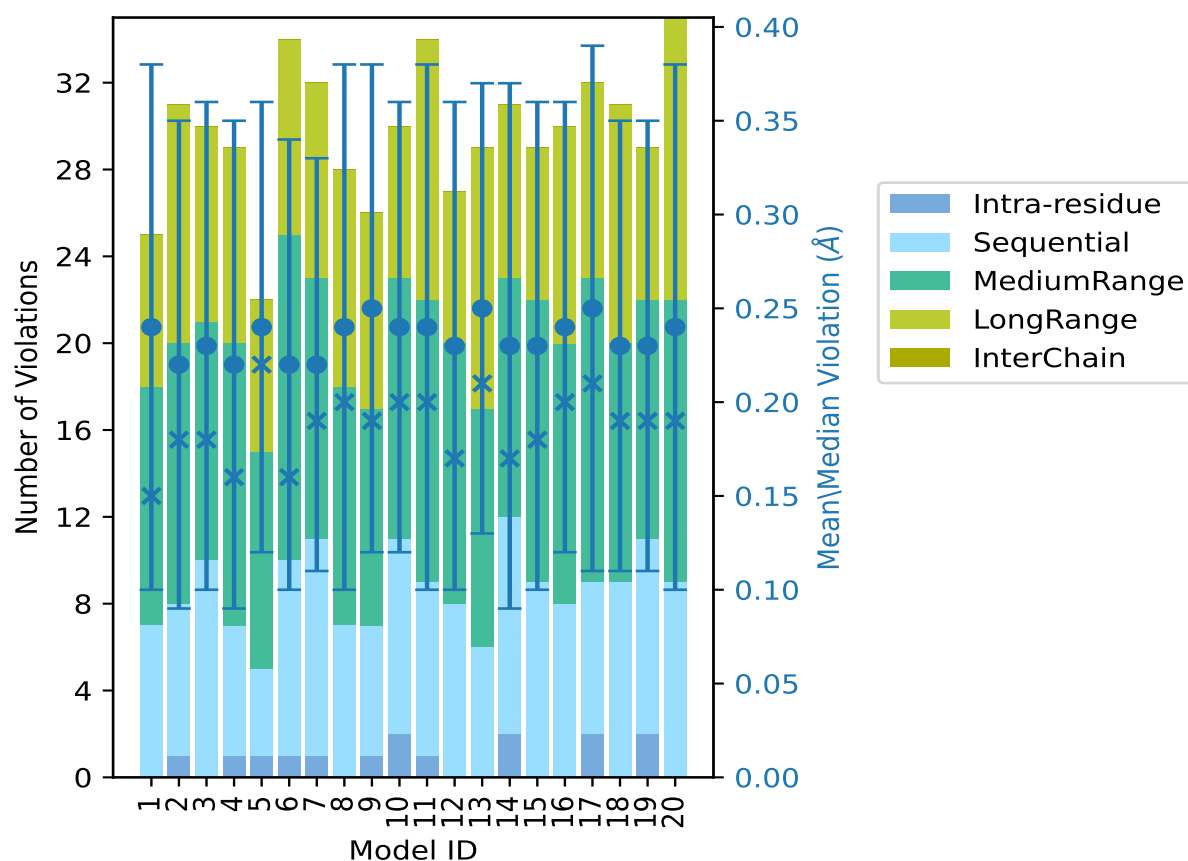
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 1                    | 8               | 13              | 12              | 0               | 34    | 0.24     | 0.63    | 0.14                | 0.2        |
| 12       | 0                    | 8               | 12              | 7               | 0               | 27    | 0.23     | 0.63    | 0.13                | 0.17       |
| 13       | 0                    | 6               | 11              | 12              | 0               | 29    | 0.25     | 0.64    | 0.12                | 0.21       |
| 14       | 2                    | 10              | 11              | 8               | 0               | 31    | 0.23     | 0.63    | 0.14                | 0.17       |
| 15       | 0                    | 9               | 13              | 7               | 0               | 29    | 0.23     | 0.58    | 0.13                | 0.18       |
| 16       | 0                    | 8               | 12              | 10              | 0               | 30    | 0.24     | 0.62    | 0.12                | 0.2        |
| 17       | 2                    | 7               | 14              | 9               | 0               | 32    | 0.25     | 0.6     | 0.14                | 0.21       |
| 18       | 0                    | 9               | 11              | 11              | 0               | 31    | 0.23     | 0.58    | 0.12                | 0.19       |
| 19       | 2                    | 9               | 11              | 7               | 0               | 29    | 0.23     | 0.63    | 0.12                | 0.19       |
| 20       | 0                    | 9               | 13              | 13              | 0               | 35    | 0.24     | 0.6     | 0.14                | 0.19       |

<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

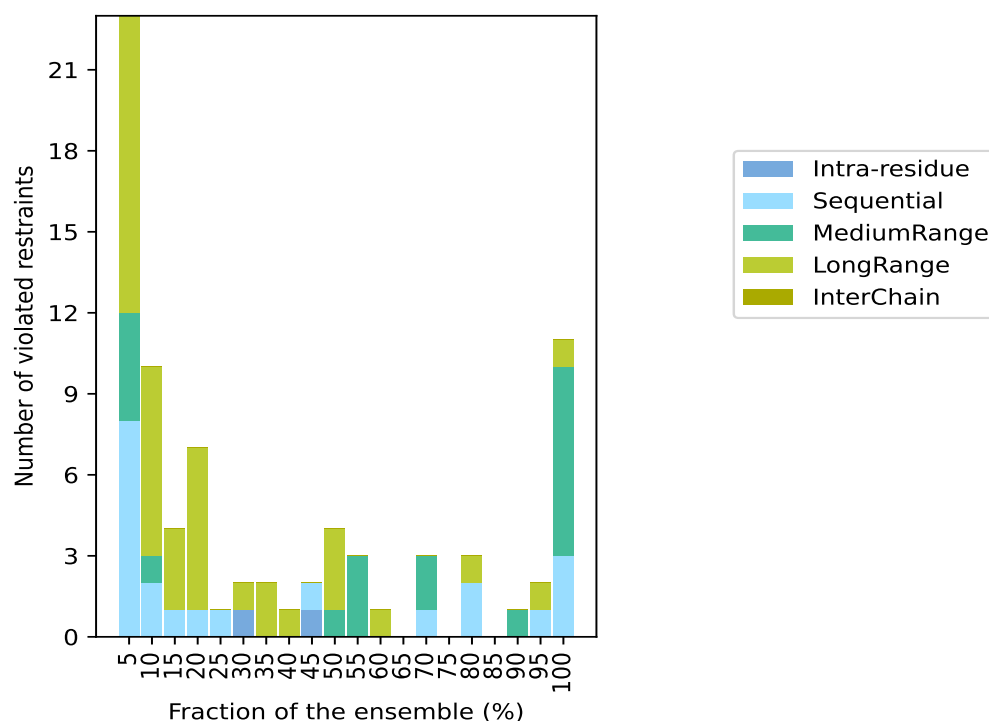
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1703(IR:277, SQ:500, MR:342, LR:584, IC:0) restraints are 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                             | 8               | 4               | 11              | 0               | 23    | 1                        | 5.0   |
| 0                             | 2               | 1               | 7               | 0               | 10    | 2                        | 10.0  |
| 0                             | 1               | 0               | 3               | 0               | 4     | 3                        | 15.0  |
| 0                             | 1               | 0               | 6               | 0               | 7     | 4                        | 20.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 5                        | 25.0  |
| 1                             | 0               | 0               | 1               | 0               | 2     | 6                        | 30.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 7                        | 35.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 8                        | 40.0  |
| 1                             | 1               | 0               | 0               | 0               | 2     | 9                        | 45.0  |
| 0                             | 0               | 1               | 3               | 0               | 4     | 10                       | 50.0  |
| 0                             | 0               | 3               | 0               | 0               | 3     | 11                       | 55.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 12                       | 60.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 13                       | 65.0  |
| 0                             | 1               | 2               | 0               | 0               | 3     | 14                       | 70.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 15                       | 75.0  |
| 0                             | 2               | 0               | 1               | 0               | 3     | 16                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 85.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 18                       | 90.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 19                       | 95.0  |
| 0                             | 3               | 7               | 1               | 0               | 11    | 20                       | 100.0 |

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

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

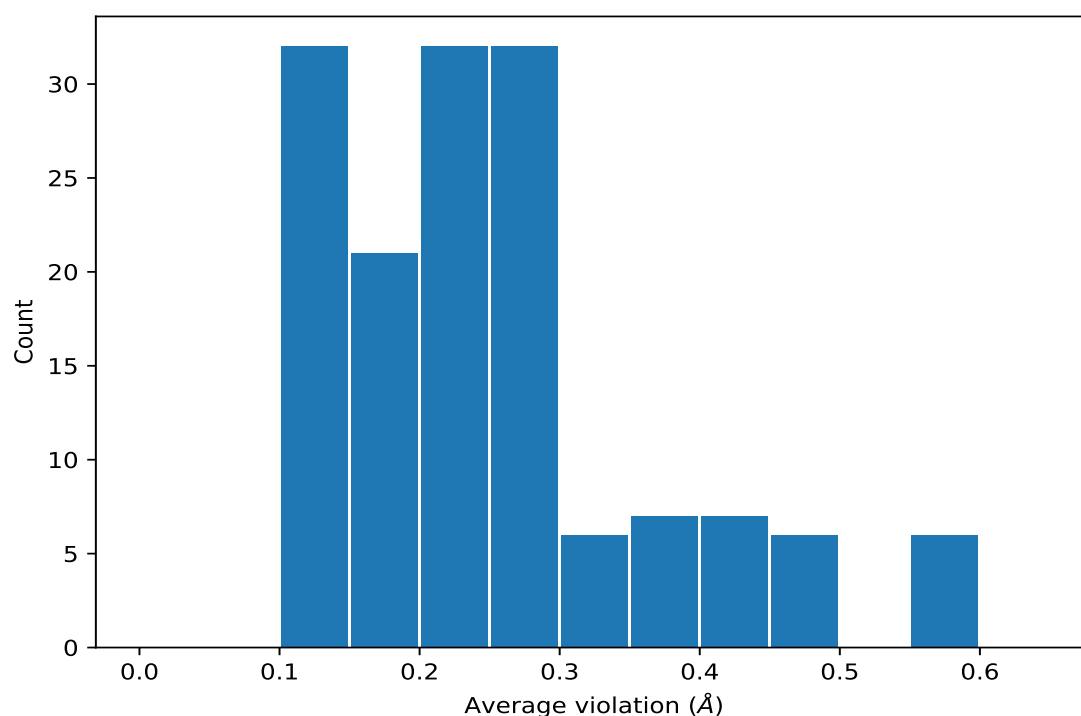
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,490)  | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD11 | 20                  | 0.6      | 0.03                | 0.6        |
| (1,490)  | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD12 | 20                  | 0.6      | 0.03                | 0.6        |
| (1,490)  | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD13 | 20                  | 0.6      | 0.03                | 0.6        |
| (1,490)  | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD11 | 20                  | 0.6      | 0.03                | 0.6        |
| (1,490)  | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD12 | 20                  | 0.6      | 0.03                | 0.6        |
| (1,490)  | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD13 | 20                  | 0.6      | 0.03                | 0.6        |
| (1,1291) | 1:99:A:ALA:H   | 1:98:A:LYS:HA   | 20                  | 0.44     | 0.03                | 0.44       |
| (1,1197) | 1:81:A:VAL:H   | 1:79:A:VAL:HG11 | 20                  | 0.37     | 0.07                | 0.38       |
| (1,1197) | 1:81:A:VAL:H   | 1:79:A:VAL:HG12 | 20                  | 0.37     | 0.07                | 0.38       |
| (1,1197) | 1:81:A:VAL:H   | 1:79:A:VAL:HG13 | 20                  | 0.37     | 0.07                | 0.38       |
| (1,954)  | 1:43:A:GLU:H   | 1:44:A:ARG:HA   | 20                  | 0.28     | 0.04                | 0.28       |
| (1,1015) | 1:56:A:TYR:H   | 1:57:A:MET:HB2  | 20                  | 0.27     | 0.03                | 0.28       |
| (1,792)  | 1:120:A:VAL:HA | 1:57:A:MET:HA   | 20                  | 0.23     | 0.04                | 0.23       |
| (1,1126) | 1:71:A:LEU:H   | 1:69:A:ARG:HB2  | 20                  | 0.22     | 0.05                | 0.24       |
| (1,551)  | 1:96:A:GLU:HA  | 1:99:A:ALA:HA   | 20                  | 0.2      | 0.03                | 0.19       |
| (1,1374) | 1:110:A:LEU:H  | 1:114:A:SER:HB3 | 20                  | 0.17     | 0.02                | 0.17       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA    | 20                  | 0.16     | 0.01                | 0.16       |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 20                  | 0.15     | 0.03                | 0.15       |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA    | 19                  | 0.39     | 0.09                | 0.43       |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2   | 19                  | 0.16     | 0.04                | 0.14       |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3   | 19                  | 0.16     | 0.04                | 0.14       |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2   | 19                  | 0.16     | 0.04                | 0.14       |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3   | 19                  | 0.16     | 0.04                | 0.14       |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2   | 19                  | 0.16     | 0.04                | 0.14       |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3   | 19                  | 0.16     | 0.04                | 0.14       |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 18                  | 0.21     | 0.05                | 0.2        |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1   | 16                  | 0.43     | 0.13                | 0.47       |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2   | 16                  | 0.43     | 0.13                | 0.47       |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1   | 16                  | 0.43     | 0.13                | 0.47       |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2   | 16                  | 0.43     | 0.13                | 0.47       |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1   | 16                  | 0.43     | 0.13                | 0.47       |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2   | 16                  | 0.43     | 0.13                | 0.47       |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA   | 16                  | 0.18     | 0.05                | 0.18       |
| (1,957)  | 1:44:A:ARG:H    | 1:43:A:GLU:H     | 16                  | 0.14     | 0.02                | 0.13       |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB   | 14                  | 0.14     | 0.03                | 0.14       |
| (1,478)  | 1:87:A:THR:HB   | 1:83:A:LEU:HG    | 14                  | 0.13     | 0.02                | 0.14       |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA    | 14                  | 0.12     | 0.02                | 0.11       |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG12 | 12                  | 0.24     | 0.11                | 0.22       |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG13 | 12                  | 0.24     | 0.11                | 0.22       |
| (1,903)  | 1:32:A:GLY:H    | 1:34:A:GLU:H     | 11                  | 0.2      | 0.06                | 0.21       |
| (1,1066) | 1:63:A:ALA:H    | 1:61:A:GLU:HB2   | 11                  | 0.12     | 0.02                | 0.12       |
| (1,1071) | 1:63:A:ALA:H    | 1:65:A:VAL:HB    | 11                  | 0.12     | 0.01                | 0.12       |
| (1,438)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HA    | 10                  | 0.38     | 0.1                 | 0.4        |
| (1,438)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HA    | 10                  | 0.38     | 0.1                 | 0.4        |
| (1,438)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HA    | 10                  | 0.38     | 0.1                 | 0.4        |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD2  | 10                  | 0.3      | 0.09                | 0.33       |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD3  | 10                  | 0.3      | 0.09                | 0.33       |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD2  | 10                  | 0.3      | 0.09                | 0.33       |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD3  | 10                  | 0.3      | 0.09                | 0.33       |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD2  | 10                  | 0.3      | 0.09                | 0.33       |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD3  | 10                  | 0.3      | 0.09                | 0.33       |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG2   | 10                  | 0.29     | 0.11                | 0.3        |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG3   | 10                  | 0.29     | 0.11                | 0.3        |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG2   | 10                  | 0.29     | 0.11                | 0.3        |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG3   | 10                  | 0.29     | 0.11                | 0.3        |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG2   | 10                  | 0.29     | 0.11                | 0.3        |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG3   | 10                  | 0.29     | 0.11                | 0.3        |
| (1,930)  | 1:38:A:ILE:H    | 1:36:A:VAL:HA    | 10                  | 0.15     | 0.04                | 0.15       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1534) | 1:57:A:MET:H    | 1:57:A:MET:HB2   | 9                   | 0.12     | 0.01                | 0.11       |
| (1,1492) | 1:124:A:ILE:H   | 1:123:A:LEU:HG   | 9                   | 0.11     | 0.01                | 0.11       |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE1  | 8                   | 0.25     | 0.09                | 0.22       |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE2  | 8                   | 0.25     | 0.09                | 0.22       |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE1  | 8                   | 0.25     | 0.09                | 0.22       |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE2  | 8                   | 0.25     | 0.09                | 0.22       |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD11 | 7                   | 0.23     | 0.05                | 0.21       |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD12 | 7                   | 0.23     | 0.05                | 0.21       |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD13 | 7                   | 0.23     | 0.05                | 0.21       |
| (1,426)  | 1:79:A:VAL:HG21 | 1:92:A:ILE:HG21  | 7                   | 0.13     | 0.02                | 0.13       |
| (1,426)  | 1:79:A:VAL:HG21 | 1:92:A:ILE:HG22  | 7                   | 0.13     | 0.02                | 0.13       |
| (1,426)  | 1:79:A:VAL:HG21 | 1:92:A:ILE:HG23  | 7                   | 0.13     | 0.02                | 0.13       |
| (1,426)  | 1:79:A:VAL:HG22 | 1:92:A:ILE:HG21  | 7                   | 0.13     | 0.02                | 0.13       |
| (1,426)  | 1:79:A:VAL:HG22 | 1:92:A:ILE:HG22  | 7                   | 0.13     | 0.02                | 0.13       |
| (1,426)  | 1:79:A:VAL:HG22 | 1:92:A:ILE:HG23  | 7                   | 0.13     | 0.02                | 0.13       |
| (1,426)  | 1:79:A:VAL:HG23 | 1:92:A:ILE:HG21  | 7                   | 0.13     | 0.02                | 0.13       |
| (1,426)  | 1:79:A:VAL:HG23 | 1:92:A:ILE:HG22  | 7                   | 0.13     | 0.02                | 0.13       |
| (1,426)  | 1:79:A:VAL:HG23 | 1:92:A:ILE:HG23  | 7                   | 0.13     | 0.02                | 0.13       |
| (1,439)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HG2   | 6                   | 0.2      | 0.05                | 0.2        |
| (1,439)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HG3   | 6                   | 0.2      | 0.05                | 0.2        |
| (1,439)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HG2   | 6                   | 0.2      | 0.05                | 0.2        |
| (1,439)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HG3   | 6                   | 0.2      | 0.05                | 0.2        |
| (1,439)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HG2   | 6                   | 0.2      | 0.05                | 0.2        |
| (1,439)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HG3   | 6                   | 0.2      | 0.05                | 0.2        |
| (1,1731) | 1:52:A:ILE:H    | 1:52:A:ILE:HG12  | 6                   | 0.18     | 0.08                | 0.15       |
| (1,1731) | 1:52:A:ILE:H    | 1:52:A:ILE:HG13  | 6                   | 0.18     | 0.08                | 0.15       |
| (1,1339) | 1:107:A:ARG:HE  | 1:108:A:ARG:H    | 5                   | 0.15     | 0.03                | 0.16       |
| (1,60)   | 1:36:A:VAL:HG21 | 1:60:A:TYR:HE1   | 4                   | 0.46     | 0.08                | 0.48       |
| (1,60)   | 1:36:A:VAL:HG21 | 1:60:A:TYR:HE2   | 4                   | 0.46     | 0.08                | 0.48       |
| (1,60)   | 1:36:A:VAL:HG22 | 1:60:A:TYR:HE1   | 4                   | 0.46     | 0.08                | 0.48       |
| (1,60)   | 1:36:A:VAL:HG22 | 1:60:A:TYR:HE2   | 4                   | 0.46     | 0.08                | 0.48       |
| (1,60)   | 1:36:A:VAL:HG23 | 1:60:A:TYR:HE1   | 4                   | 0.46     | 0.08                | 0.48       |
| (1,60)   | 1:36:A:VAL:HG23 | 1:60:A:TYR:HE2   | 4                   | 0.46     | 0.08                | 0.48       |
| (1,445)  | 1:81:A:VAL:HG21 | 1:95:A:LYS:HB2   | 4                   | 0.3      | 0.08                | 0.32       |
| (1,445)  | 1:81:A:VAL:HG21 | 1:95:A:LYS:HB3   | 4                   | 0.3      | 0.08                | 0.32       |
| (1,445)  | 1:81:A:VAL:HG22 | 1:95:A:LYS:HB2   | 4                   | 0.3      | 0.08                | 0.32       |
| (1,445)  | 1:81:A:VAL:HG22 | 1:95:A:LYS:HB3   | 4                   | 0.3      | 0.08                | 0.32       |
| (1,445)  | 1:81:A:VAL:HG23 | 1:95:A:LYS:HB2   | 4                   | 0.3      | 0.08                | 0.32       |
| (1,445)  | 1:81:A:VAL:HG23 | 1:95:A:LYS:HB3   | 4                   | 0.3      | 0.08                | 0.32       |
| (1,117)  | 1:41:A:SER:HA   | 1:105:A:ILE:HG12 | 4                   | 0.28     | 0.09                | 0.22       |
| (1,117)  | 1:41:A:SER:HA   | 1:105:A:ILE:HG13 | 4                   | 0.28     | 0.09                | 0.22       |
| (1,130)  | 1:44:A:ARG:HA   | 1:105:A:ILE:HD11 | 4                   | 0.21     | 0.07                | 0.22       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,130) | 1:44:A:ARG:HA    | 1:105:A:ILE:HD12 | 4                   | 0.21     | 0.07                | 0.22       |
| (1,130) | 1:44:A:ARG:HA    | 1:105:A:ILE:HD13 | 4                   | 0.21     | 0.07                | 0.22       |
| (1,891) | 1:27:A:ASN:H     | 1:26:A:GLU:HA    | 4                   | 0.2      | 0.09                | 0.16       |
| (1,804) | 1:120:A:VAL:HG21 | 1:57:A:MET:HE1   | 4                   | 0.16     | 0.06                | 0.14       |
| (1,804) | 1:120:A:VAL:HG21 | 1:57:A:MET:HE2   | 4                   | 0.16     | 0.06                | 0.14       |
| (1,804) | 1:120:A:VAL:HG21 | 1:57:A:MET:HE3   | 4                   | 0.16     | 0.06                | 0.14       |
| (1,804) | 1:120:A:VAL:HG22 | 1:57:A:MET:HE1   | 4                   | 0.16     | 0.06                | 0.14       |
| (1,804) | 1:120:A:VAL:HG22 | 1:57:A:MET:HE2   | 4                   | 0.16     | 0.06                | 0.14       |
| (1,804) | 1:120:A:VAL:HG22 | 1:57:A:MET:HE3   | 4                   | 0.16     | 0.06                | 0.14       |
| (1,804) | 1:120:A:VAL:HG23 | 1:57:A:MET:HE1   | 4                   | 0.16     | 0.06                | 0.14       |
| (1,804) | 1:120:A:VAL:HG23 | 1:57:A:MET:HE2   | 4                   | 0.16     | 0.06                | 0.14       |
| (1,804) | 1:120:A:VAL:HG23 | 1:57:A:MET:HE3   | 4                   | 0.16     | 0.06                | 0.14       |
| (1,206) | 1:55:A:PRO:HB2   | 1:118:A:TRP:HZ3  | 4                   | 0.14     | 0.02                | 0.13       |
| (1,206) | 1:55:A:PRO:HB3   | 1:118:A:TRP:HZ3  | 4                   | 0.14     | 0.02                | 0.13       |
| (1,918) | 1:36:A:VAL:H     | 1:35:A:ASN:HB2   | 3                   | 0.15     | 0.03                | 0.16       |
| (1,998) | 1:53:A:THR:H     | 1:118:A:TRP:HH2  | 3                   | 0.12     | 0.01                | 0.12       |
| (1,199) | 1:55:A:PRO:HA    | 1:118:A:TRP:HZ2  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,608) | 1:105:A:ILE:HB   | 1:117:A:ASP:HA   | 3                   | 0.11     | 0.01                | 0.12       |
| (1,132) | 1:44:A:ARG:HD2   | 1:105:A:ILE:HD11 | 2                   | 0.33     | 0.07                | 0.33       |
| (1,132) | 1:44:A:ARG:HD2   | 1:105:A:ILE:HD12 | 2                   | 0.33     | 0.07                | 0.33       |
| (1,132) | 1:44:A:ARG:HD2   | 1:105:A:ILE:HD13 | 2                   | 0.33     | 0.07                | 0.33       |
| (1,132) | 1:44:A:ARG:HD3   | 1:105:A:ILE:HD11 | 2                   | 0.33     | 0.07                | 0.33       |
| (1,132) | 1:44:A:ARG:HD3   | 1:105:A:ILE:HD12 | 2                   | 0.33     | 0.07                | 0.33       |
| (1,132) | 1:44:A:ARG:HD3   | 1:105:A:ILE:HD13 | 2                   | 0.33     | 0.07                | 0.33       |
| (1,140) | 1:45:A:PRO:HD2   | 1:105:A:ILE:HD11 | 2                   | 0.28     | 0.07                | 0.28       |
| (1,140) | 1:45:A:PRO:HD2   | 1:105:A:ILE:HD12 | 2                   | 0.28     | 0.07                | 0.28       |
| (1,140) | 1:45:A:PRO:HD2   | 1:105:A:ILE:HD13 | 2                   | 0.28     | 0.07                | 0.28       |
| (1,140) | 1:45:A:PRO:HD3   | 1:105:A:ILE:HD11 | 2                   | 0.28     | 0.07                | 0.28       |
| (1,140) | 1:45:A:PRO:HD3   | 1:105:A:ILE:HD12 | 2                   | 0.28     | 0.07                | 0.28       |
| (1,140) | 1:45:A:PRO:HD3   | 1:105:A:ILE:HD13 | 2                   | 0.28     | 0.07                | 0.28       |
| (1,629) | 1:106:A:ILE:HD11 | 1:57:A:MET:HE1   | 2                   | 0.22     | 0.12                | 0.22       |
| (1,629) | 1:106:A:ILE:HD11 | 1:57:A:MET:HE2   | 2                   | 0.22     | 0.12                | 0.22       |
| (1,629) | 1:106:A:ILE:HD11 | 1:57:A:MET:HE3   | 2                   | 0.22     | 0.12                | 0.22       |
| (1,629) | 1:106:A:ILE:HD12 | 1:57:A:MET:HE1   | 2                   | 0.22     | 0.12                | 0.22       |
| (1,629) | 1:106:A:ILE:HD12 | 1:57:A:MET:HE2   | 2                   | 0.22     | 0.12                | 0.22       |
| (1,629) | 1:106:A:ILE:HD12 | 1:57:A:MET:HE3   | 2                   | 0.22     | 0.12                | 0.22       |
| (1,629) | 1:106:A:ILE:HD13 | 1:57:A:MET:HE1   | 2                   | 0.22     | 0.12                | 0.22       |
| (1,629) | 1:106:A:ILE:HD13 | 1:57:A:MET:HE2   | 2                   | 0.22     | 0.12                | 0.22       |
| (1,629) | 1:106:A:ILE:HD13 | 1:57:A:MET:HE3   | 2                   | 0.22     | 0.12                | 0.22       |
| (1,849) | 1:125:A:ILE:HD11 | 1:57:A:MET:HB3   | 2                   | 0.22     | 0.05                | 0.22       |
| (1,849) | 1:125:A:ILE:HD12 | 1:57:A:MET:HB3   | 2                   | 0.22     | 0.05                | 0.22       |
| (1,849) | 1:125:A:ILE:HD13 | 1:57:A:MET:HB3   | 2                   | 0.22     | 0.05                | 0.22       |

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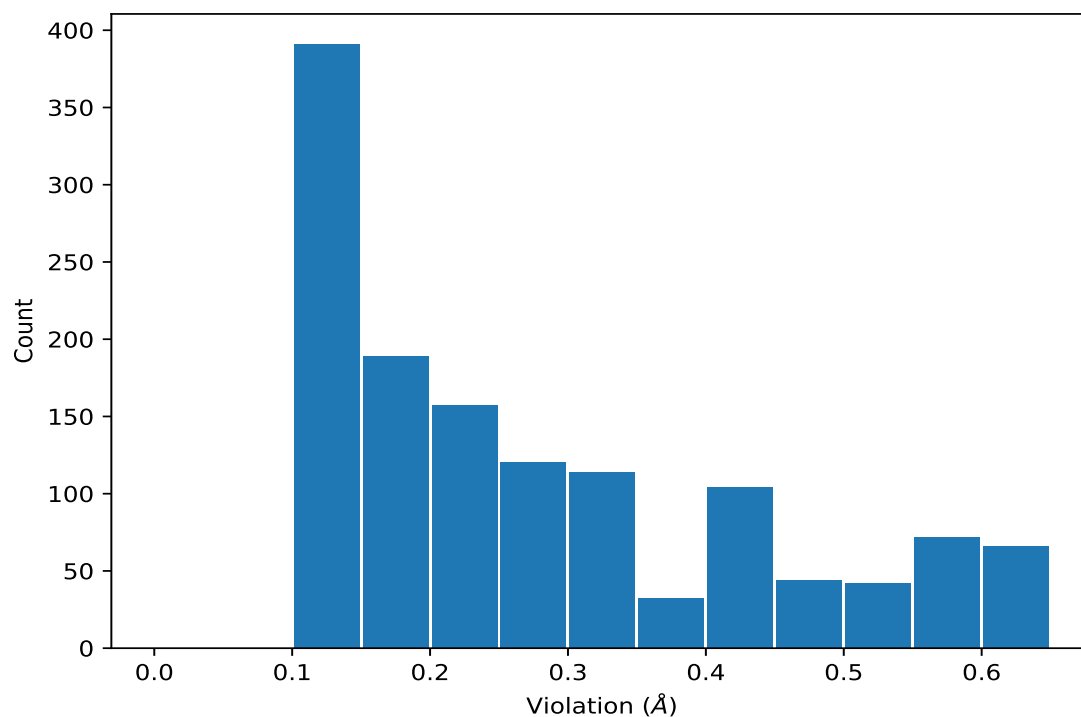
| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,898) | 1:30:A:GLU:H    | 1:29:A:GLU:HA   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,870) | 1:13:A:PHE:H    | 1:12:A:ASP:HA   | 2                   | 0.14     | 0.01                | 0.14       |
| (1,783) | 1:118:A:TRP:HZ3 | 1:122:A:GLU:HA  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,748) | 1:118:A:TRP:HA  | 1:106:A:ILE:HB  | 2                   | 0.12     | 0.01                | 0.12       |
| (2,27)  | 1:68:A:THR:O    | 1:72:A:GLN:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,978) | 1:51:A:ARG:HE   | 1:118:A:TRP:HH2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,939) | 1:39:A:LEU:H    | 1:104:A:ILE:HA  | 2                   | 0.1      | 0.0                 | 0.1        |

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

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

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

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



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

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



| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD11 | 13       | 0.64          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD12 | 13       | 0.64          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD13 | 13       | 0.64          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD11 | 13       | 0.64          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD12 | 13       | 0.64          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD13 | 13       | 0.64          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD11 | 8        | 0.63          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD12 | 8        | 0.63          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD13 | 8        | 0.63          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD11 | 8        | 0.63          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD12 | 8        | 0.63          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD13 | 8        | 0.63          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD11 | 12       | 0.63          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD12 | 12       | 0.63          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD13 | 12       | 0.63          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD11 | 12       | 0.63          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD12 | 12       | 0.63          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD13 | 12       | 0.63          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD11 | 14       | 0.63          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD12 | 14       | 0.63          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD13 | 14       | 0.63          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD11 | 14       | 0.63          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD12 | 14       | 0.63          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD13 | 14       | 0.63          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD11 | 19       | 0.63          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD12 | 19       | 0.63          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD13 | 19       | 0.63          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD11 | 19       | 0.63          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD12 | 19       | 0.63          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD13 | 19       | 0.63          |
| (1,52)  | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1  | 11       | 0.63          |
| (1,52)  | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2  | 11       | 0.63          |
| (1,52)  | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1  | 11       | 0.63          |
| (1,52)  | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2  | 11       | 0.63          |
| (1,52)  | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1  | 11       | 0.63          |
| (1,52)  | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2  | 11       | 0.63          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD11 | 11       | 0.62          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD12 | 11       | 0.62          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD13 | 11       | 0.62          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD11 | 11       | 0.62          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD12 | 11       | 0.62          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD13 | 11       | 0.62          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD11 | 16       | 0.62          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD12 | 16       | 0.62          |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD13 | 16       | 0.62          |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD11 | 16       | 0.62          |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD12 | 16       | 0.62          |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD13 | 16       | 0.62          |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD11 | 3        | 0.61          |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD12 | 3        | 0.61          |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD13 | 3        | 0.61          |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD11 | 3        | 0.61          |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD12 | 3        | 0.61          |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD13 | 3        | 0.61          |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD11 | 4        | 0.61          |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD12 | 4        | 0.61          |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD13 | 4        | 0.61          |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD11 | 4        | 0.61          |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD12 | 4        | 0.61          |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD13 | 4        | 0.61          |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD11 | 9        | 0.61          |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD12 | 9        | 0.61          |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD13 | 9        | 0.61          |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD11 | 9        | 0.61          |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD12 | 9        | 0.61          |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD13 | 9        | 0.61          |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD11 | 2        | 0.6           |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD12 | 2        | 0.6           |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD13 | 2        | 0.6           |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD11 | 2        | 0.6           |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD12 | 2        | 0.6           |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD13 | 2        | 0.6           |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD11 | 6        | 0.6           |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD12 | 6        | 0.6           |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD13 | 6        | 0.6           |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD11 | 6        | 0.6           |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD12 | 6        | 0.6           |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD13 | 6        | 0.6           |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD11 | 17       | 0.6           |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD12 | 17       | 0.6           |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD13 | 17       | 0.6           |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD11 | 17       | 0.6           |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD12 | 17       | 0.6           |
| (1,490) | 1:88:A:ASP:HB3 | 1:91:A:LEU:HD13 | 17       | 0.6           |
| (1,490) | 1:88:A:ASP:HB2 | 1:91:A:LEU:HD11 | 20       | 0.6           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD12 | 20       | 0.6           |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD13 | 20       | 0.6           |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD11 | 20       | 0.6           |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD12 | 20       | 0.6           |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD13 | 20       | 0.6           |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD11 | 7        | 0.59          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD12 | 7        | 0.59          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD13 | 7        | 0.59          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD11 | 7        | 0.59          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD12 | 7        | 0.59          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD13 | 7        | 0.59          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD11 | 1        | 0.58          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD12 | 1        | 0.58          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD13 | 1        | 0.58          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD11 | 1        | 0.58          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD12 | 1        | 0.58          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD13 | 1        | 0.58          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD11 | 18       | 0.58          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD12 | 18       | 0.58          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD13 | 18       | 0.58          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD11 | 18       | 0.58          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD12 | 18       | 0.58          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD13 | 18       | 0.58          |
| (1,52)  | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1  | 15       | 0.58          |
| (1,52)  | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2  | 15       | 0.58          |
| (1,52)  | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1  | 15       | 0.58          |
| (1,52)  | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2  | 15       | 0.58          |
| (1,52)  | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1  | 15       | 0.58          |
| (1,52)  | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2  | 15       | 0.58          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD11 | 10       | 0.57          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD12 | 10       | 0.57          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD13 | 10       | 0.57          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD11 | 10       | 0.57          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD12 | 10       | 0.57          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD13 | 10       | 0.57          |
| (1,52)  | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1  | 2        | 0.57          |
| (1,52)  | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2  | 2        | 0.57          |
| (1,52)  | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1  | 2        | 0.57          |
| (1,52)  | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2  | 2        | 0.57          |
| (1,52)  | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1  | 2        | 0.57          |
| (1,52)  | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2  | 2        | 0.57          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD11 | 5        | 0.56          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD12  | 5        | 0.56          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD13  | 5        | 0.56          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD11  | 5        | 0.56          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD12  | 5        | 0.56          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD13  | 5        | 0.56          |
| (1,52)  | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1   | 17       | 0.56          |
| (1,52)  | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2   | 17       | 0.56          |
| (1,52)  | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1   | 17       | 0.56          |
| (1,52)  | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2   | 17       | 0.56          |
| (1,52)  | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1   | 17       | 0.56          |
| (1,52)  | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2   | 17       | 0.56          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD11  | 15       | 0.54          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD12  | 15       | 0.54          |
| (1,490) | 1:88:A:ASP:HB2  | 1:91:A:LEU:HD13  | 15       | 0.54          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD11  | 15       | 0.54          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD12  | 15       | 0.54          |
| (1,490) | 1:88:A:ASP:HB3  | 1:91:A:LEU:HD13  | 15       | 0.54          |
| (1,60)  | 1:36:A:VAL:HG21 | 1:60:A:TYR:HE1   | 20       | 0.54          |
| (1,60)  | 1:36:A:VAL:HG21 | 1:60:A:TYR:HE2   | 20       | 0.54          |
| (1,60)  | 1:36:A:VAL:HG22 | 1:60:A:TYR:HE1   | 20       | 0.54          |
| (1,60)  | 1:36:A:VAL:HG22 | 1:60:A:TYR:HE2   | 20       | 0.54          |
| (1,60)  | 1:36:A:VAL:HG23 | 1:60:A:TYR:HE1   | 20       | 0.54          |
| (1,60)  | 1:36:A:VAL:HG23 | 1:60:A:TYR:HE2   | 20       | 0.54          |
| (1,121) | 1:41:A:SER:HB3  | 1:105:A:ILE:HG12 | 20       | 0.53          |
| (1,121) | 1:41:A:SER:HB3  | 1:105:A:ILE:HG13 | 20       | 0.53          |
| (1,60)  | 1:36:A:VAL:HG21 | 1:60:A:TYR:HE1   | 1        | 0.53          |
| (1,60)  | 1:36:A:VAL:HG21 | 1:60:A:TYR:HE2   | 1        | 0.53          |
| (1,60)  | 1:36:A:VAL:HG22 | 1:60:A:TYR:HE1   | 1        | 0.53          |
| (1,60)  | 1:36:A:VAL:HG22 | 1:60:A:TYR:HE2   | 1        | 0.53          |
| (1,60)  | 1:36:A:VAL:HG23 | 1:60:A:TYR:HE1   | 1        | 0.53          |
| (1,60)  | 1:36:A:VAL:HG23 | 1:60:A:TYR:HE2   | 1        | 0.53          |
| (1,52)  | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1   | 14       | 0.53          |
| (1,52)  | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2   | 14       | 0.53          |
| (1,52)  | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1   | 14       | 0.53          |
| (1,52)  | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2   | 14       | 0.53          |
| (1,52)  | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1   | 14       | 0.53          |
| (1,52)  | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2   | 14       | 0.53          |
| (1,734) | 1:116:A:GLU:HG2 | 1:51:A:ARG:HG2   | 11       | 0.52          |
| (1,734) | 1:116:A:GLU:HG2 | 1:51:A:ARG:HG3   | 11       | 0.52          |
| (1,734) | 1:116:A:GLU:HG3 | 1:51:A:ARG:HG2   | 11       | 0.52          |
| (1,734) | 1:116:A:GLU:HG3 | 1:51:A:ARG:HG3   | 11       | 0.52          |
| (1,438) | 1:81:A:VAL:HG11 | 1:96:A:GLU:HA    | 9        | 0.5           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,438)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HA   | 9        | 0.5           |
| (1,438)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HA   | 9        | 0.5           |
| (1,438)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HA   | 17       | 0.5           |
| (1,438)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HA   | 17       | 0.5           |
| (1,438)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HA   | 17       | 0.5           |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1  | 4        | 0.5           |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2  | 4        | 0.5           |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1  | 4        | 0.5           |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2  | 4        | 0.5           |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1  | 4        | 0.5           |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2  | 4        | 0.5           |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA   | 3        | 0.49          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA   | 20       | 0.49          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1  | 16       | 0.49          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2  | 16       | 0.49          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1  | 16       | 0.49          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2  | 16       | 0.49          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1  | 16       | 0.49          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2  | 16       | 0.49          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11 | 3        | 0.48          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12 | 3        | 0.48          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13 | 3        | 0.48          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA   | 8        | 0.48          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1  | 13       | 0.48          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2  | 13       | 0.48          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1  | 13       | 0.48          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2  | 13       | 0.48          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1  | 13       | 0.48          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2  | 13       | 0.48          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA   | 12       | 0.47          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11 | 6        | 0.47          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12 | 6        | 0.47          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13 | 6        | 0.47          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA   | 10       | 0.47          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA   | 16       | 0.47          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA   | 17       | 0.47          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA   | 2        | 0.46          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA   | 5        | 0.46          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA   | 14       | 0.46          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA   | 3        | 0.46          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA   | 9        | 0.46          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA   | 15       | 0.46          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1   | 8        | 0.46          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2   | 8        | 0.46          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1   | 8        | 0.46          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2   | 8        | 0.46          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1   | 8        | 0.46          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2   | 8        | 0.46          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA    | 1        | 0.45          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA    | 4        | 0.45          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA    | 10       | 0.45          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA    | 15       | 0.45          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11  | 12       | 0.45          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12  | 12       | 0.45          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13  | 12       | 0.45          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA    | 8        | 0.44          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA    | 7        | 0.44          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA    | 14       | 0.44          |
| (1,438)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HA    | 10       | 0.44          |
| (1,438)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HA    | 10       | 0.44          |
| (1,438)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HA    | 10       | 0.44          |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG2   | 14       | 0.44          |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG3   | 14       | 0.44          |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG2   | 14       | 0.44          |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG3   | 14       | 0.44          |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG2   | 14       | 0.44          |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG3   | 14       | 0.44          |
| (1,117)  | 1:41:A:SER:HA   | 1:105:A:ILE:HG12 | 4        | 0.44          |
| (1,117)  | 1:41:A:SER:HA   | 1:105:A:ILE:HG13 | 4        | 0.44          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA    | 9        | 0.43          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA    | 18       | 0.43          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11  | 1        | 0.43          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12  | 1        | 0.43          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13  | 1        | 0.43          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11  | 2        | 0.43          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12  | 2        | 0.43          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13  | 2        | 0.43          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11  | 18       | 0.43          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12  | 18       | 0.43          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13  | 18       | 0.43          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA    | 1        | 0.43          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA    | 20       | 0.43          |
| (1,60)   | 1:36:A:VAL:HG21 | 1:60:A:TYR:HE1   | 5        | 0.43          |
| (1,60)   | 1:36:A:VAL:HG21 | 1:60:A:TYR:HE2   | 5        | 0.43          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,60)   | 1:36:A:VAL:HG22 | 1:60:A:TYR:HE1  | 5        | 0.43          |
| (1,60)   | 1:36:A:VAL:HG22 | 1:60:A:TYR:HE2  | 5        | 0.43          |
| (1,60)   | 1:36:A:VAL:HG23 | 1:60:A:TYR:HE1  | 5        | 0.43          |
| (1,60)   | 1:36:A:VAL:HG23 | 1:60:A:TYR:HE2  | 5        | 0.43          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA   | 6        | 0.42          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA   | 11       | 0.42          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11 | 8        | 0.42          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12 | 8        | 0.42          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13 | 8        | 0.42          |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD2 | 18       | 0.42          |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD3 | 18       | 0.42          |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD2 | 18       | 0.42          |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD3 | 18       | 0.42          |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD2 | 18       | 0.42          |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD3 | 18       | 0.42          |
| (1,438)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HA   | 18       | 0.42          |
| (1,438)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HA   | 18       | 0.42          |
| (1,438)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HA   | 18       | 0.42          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA   | 13       | 0.41          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA   | 16       | 0.41          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11 | 19       | 0.41          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12 | 19       | 0.41          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13 | 19       | 0.41          |
| (1,445)  | 1:81:A:VAL:HG21 | 1:95:A:LYS:HB2  | 20       | 0.41          |
| (1,445)  | 1:81:A:VAL:HG21 | 1:95:A:LYS:HB3  | 20       | 0.41          |
| (1,445)  | 1:81:A:VAL:HG22 | 1:95:A:LYS:HB2  | 20       | 0.41          |
| (1,445)  | 1:81:A:VAL:HG22 | 1:95:A:LYS:HB3  | 20       | 0.41          |
| (1,445)  | 1:81:A:VAL:HG23 | 1:95:A:LYS:HB2  | 20       | 0.41          |
| (1,445)  | 1:81:A:VAL:HG23 | 1:95:A:LYS:HB3  | 20       | 0.41          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11 | 10       | 0.4           |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12 | 10       | 0.4           |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13 | 10       | 0.4           |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11 | 14       | 0.4           |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12 | 14       | 0.4           |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13 | 14       | 0.4           |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD2 | 20       | 0.4           |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD3 | 20       | 0.4           |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD2 | 20       | 0.4           |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD3 | 20       | 0.4           |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD2 | 20       | 0.4           |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD3 | 20       | 0.4           |
| (1,438)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HA   | 11       | 0.4           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,438)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HA    | 11       | 0.4           |
| (1,438)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HA    | 11       | 0.4           |
| (1,438)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HA    | 13       | 0.4           |
| (1,438)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HA    | 13       | 0.4           |
| (1,438)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HA    | 13       | 0.4           |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG2   | 17       | 0.4           |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG3   | 17       | 0.4           |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG2   | 17       | 0.4           |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG3   | 17       | 0.4           |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG2   | 17       | 0.4           |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG3   | 17       | 0.4           |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG2   | 19       | 0.4           |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG3   | 19       | 0.4           |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG2   | 19       | 0.4           |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG3   | 19       | 0.4           |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG2   | 19       | 0.4           |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG3   | 19       | 0.4           |
| (1,132)  | 1:44:A:ARG:HD2  | 1:105:A:ILE:HD11 | 15       | 0.4           |
| (1,132)  | 1:44:A:ARG:HD2  | 1:105:A:ILE:HD12 | 15       | 0.4           |
| (1,132)  | 1:44:A:ARG:HD2  | 1:105:A:ILE:HD13 | 15       | 0.4           |
| (1,132)  | 1:44:A:ARG:HD3  | 1:105:A:ILE:HD11 | 15       | 0.4           |
| (1,132)  | 1:44:A:ARG:HD3  | 1:105:A:ILE:HD12 | 15       | 0.4           |
| (1,132)  | 1:44:A:ARG:HD3  | 1:105:A:ILE:HD13 | 15       | 0.4           |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE1  | 6        | 0.4           |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE2  | 6        | 0.4           |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE1  | 6        | 0.4           |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE2  | 6        | 0.4           |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1   | 12       | 0.4           |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2   | 12       | 0.4           |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1   | 12       | 0.4           |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2   | 12       | 0.4           |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1   | 12       | 0.4           |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2   | 12       | 0.4           |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA    | 17       | 0.39          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA    | 2        | 0.39          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA    | 7        | 0.38          |
| (1,1291) | 1:99:A:ALA:H    | 1:98:A:LYS:HA    | 19       | 0.38          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1   | 6        | 0.38          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2   | 6        | 0.38          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1   | 6        | 0.38          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2   | 6        | 0.38          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1   | 6        | 0.38          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2   | 6        | 0.38          |
| (1,438)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HA    | 16       | 0.37          |
| (1,438)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HA    | 16       | 0.37          |
| (1,438)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HA    | 16       | 0.37          |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG2   | 8        | 0.37          |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG3   | 8        | 0.37          |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG2   | 8        | 0.37          |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG3   | 8        | 0.37          |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG2   | 8        | 0.37          |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG3   | 8        | 0.37          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11  | 20       | 0.36          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12  | 20       | 0.36          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13  | 20       | 0.36          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA    | 6        | 0.36          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA    | 18       | 0.36          |
| (1,954)  | 1:43:A:GLU:H    | 1:44:A:ARG:HA    | 17       | 0.36          |
| (1,896)  | 1:29:A:GLU:H    | 1:28:A:ALA:HA    | 13       | 0.36          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1   | 7        | 0.36          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2   | 7        | 0.36          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1   | 7        | 0.36          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2   | 7        | 0.36          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1   | 7        | 0.36          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2   | 7        | 0.36          |
| (1,1731) | 1:52:A:ILE:H    | 1:52:A:ILE:HG12  | 10       | 0.35          |
| (1,1731) | 1:52:A:ILE:H    | 1:52:A:ILE:HG13  | 10       | 0.35          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11  | 5        | 0.35          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12  | 5        | 0.35          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13  | 5        | 0.35          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11  | 15       | 0.35          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12  | 15       | 0.35          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13  | 15       | 0.35          |
| (1,954)  | 1:43:A:GLU:H    | 1:44:A:ARG:HA    | 4        | 0.35          |
| (1,891)  | 1:27:A:ASN:H    | 1:26:A:GLU:HA    | 19       | 0.35          |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD11 | 6        | 0.35          |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD12 | 6        | 0.35          |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD13 | 6        | 0.35          |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD2  | 16       | 0.35          |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD3  | 16       | 0.35          |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD2  | 16       | 0.35          |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD3  | 16       | 0.35          |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD2  | 16       | 0.35          |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD3  | 16       | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,60)   | 1:36:A:VAL:HG21  | 1:60:A:TYR:HE1   | 3        | 0.35          |
| (1,60)   | 1:36:A:VAL:HG21  | 1:60:A:TYR:HE2   | 3        | 0.35          |
| (1,60)   | 1:36:A:VAL:HG22  | 1:60:A:TYR:HE1   | 3        | 0.35          |
| (1,60)   | 1:36:A:VAL:HG22  | 1:60:A:TYR:HE2   | 3        | 0.35          |
| (1,60)   | 1:36:A:VAL:HG23  | 1:60:A:TYR:HE1   | 3        | 0.35          |
| (1,60)   | 1:36:A:VAL:HG23  | 1:60:A:TYR:HE2   | 3        | 0.35          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG11  | 7        | 0.34          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG12  | 7        | 0.34          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG13  | 7        | 0.34          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG11  | 9        | 0.34          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG12  | 9        | 0.34          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG13  | 9        | 0.34          |
| (1,1015) | 1:56:A:TYR:H     | 1:57:A:MET:HB2   | 12       | 0.34          |
| (1,955)  | 1:44:A:ARG:H     | 1:43:A:GLU:HA    | 11       | 0.34          |
| (1,954)  | 1:43:A:GLU:H     | 1:44:A:ARG:HA    | 11       | 0.34          |
| (1,629)  | 1:106:A:ILE:HD11 | 1:57:A:MET:HE1   | 19       | 0.34          |
| (1,629)  | 1:106:A:ILE:HD11 | 1:57:A:MET:HE2   | 19       | 0.34          |
| (1,629)  | 1:106:A:ILE:HD11 | 1:57:A:MET:HE3   | 19       | 0.34          |
| (1,629)  | 1:106:A:ILE:HD12 | 1:57:A:MET:HE1   | 19       | 0.34          |
| (1,629)  | 1:106:A:ILE:HD12 | 1:57:A:MET:HE2   | 19       | 0.34          |
| (1,629)  | 1:106:A:ILE:HD12 | 1:57:A:MET:HE3   | 19       | 0.34          |
| (1,629)  | 1:106:A:ILE:HD13 | 1:57:A:MET:HE1   | 19       | 0.34          |
| (1,629)  | 1:106:A:ILE:HD13 | 1:57:A:MET:HE2   | 19       | 0.34          |
| (1,629)  | 1:106:A:ILE:HD13 | 1:57:A:MET:HE3   | 19       | 0.34          |
| (1,442)  | 1:81:A:VAL:HG11  | 1:101:A:LYS:HD2  | 17       | 0.34          |
| (1,442)  | 1:81:A:VAL:HG11  | 1:101:A:LYS:HD3  | 17       | 0.34          |
| (1,442)  | 1:81:A:VAL:HG12  | 1:101:A:LYS:HD2  | 17       | 0.34          |
| (1,442)  | 1:81:A:VAL:HG12  | 1:101:A:LYS:HD3  | 17       | 0.34          |
| (1,442)  | 1:81:A:VAL:HG13  | 1:101:A:LYS:HD2  | 17       | 0.34          |
| (1,442)  | 1:81:A:VAL:HG13  | 1:101:A:LYS:HD3  | 17       | 0.34          |
| (1,140)  | 1:45:A:PRO:HD2   | 1:105:A:ILE:HD11 | 20       | 0.34          |
| (1,140)  | 1:45:A:PRO:HD2   | 1:105:A:ILE:HD12 | 20       | 0.34          |
| (1,140)  | 1:45:A:PRO:HD2   | 1:105:A:ILE:HD13 | 20       | 0.34          |
| (1,140)  | 1:45:A:PRO:HD3   | 1:105:A:ILE:HD11 | 20       | 0.34          |
| (1,140)  | 1:45:A:PRO:HD3   | 1:105:A:ILE:HD12 | 20       | 0.34          |
| (1,140)  | 1:45:A:PRO:HD3   | 1:105:A:ILE:HD13 | 20       | 0.34          |
| (1,121)  | 1:41:A:SER:HB3   | 1:105:A:ILE:HG12 | 8        | 0.34          |
| (1,121)  | 1:41:A:SER:HB3   | 1:105:A:ILE:HG13 | 8        | 0.34          |
| (1,954)  | 1:43:A:GLU:H     | 1:44:A:ARG:HA    | 6        | 0.33          |
| (1,954)  | 1:43:A:GLU:H     | 1:44:A:ARG:HA    | 19       | 0.33          |
| (1,792)  | 1:120:A:VAL:HA   | 1:57:A:MET:HA    | 5        | 0.33          |
| (1,442)  | 1:81:A:VAL:HG11  | 1:101:A:LYS:HD2  | 9        | 0.33          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD3 | 9        | 0.33          |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD2 | 9        | 0.33          |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD3 | 9        | 0.33          |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD2 | 9        | 0.33          |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD3 | 9        | 0.33          |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD2 | 10       | 0.33          |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD3 | 10       | 0.33          |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD2 | 10       | 0.33          |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD3 | 10       | 0.33          |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD2 | 10       | 0.33          |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD3 | 10       | 0.33          |
| (1,438)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HA   | 7        | 0.33          |
| (1,438)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HA   | 7        | 0.33          |
| (1,438)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HA   | 7        | 0.33          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11 | 13       | 0.32          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12 | 13       | 0.32          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13 | 13       | 0.32          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA   | 12       | 0.32          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA   | 19       | 0.32          |
| (1,445)  | 1:81:A:VAL:HG21 | 1:95:A:LYS:HB2  | 16       | 0.32          |
| (1,445)  | 1:81:A:VAL:HG21 | 1:95:A:LYS:HB3  | 16       | 0.32          |
| (1,445)  | 1:81:A:VAL:HG22 | 1:95:A:LYS:HB2  | 16       | 0.32          |
| (1,445)  | 1:81:A:VAL:HG22 | 1:95:A:LYS:HB3  | 16       | 0.32          |
| (1,445)  | 1:81:A:VAL:HG23 | 1:95:A:LYS:HB2  | 16       | 0.32          |
| (1,445)  | 1:81:A:VAL:HG23 | 1:95:A:LYS:HB3  | 16       | 0.32          |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG2  | 9        | 0.32          |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG3  | 9        | 0.32          |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG2  | 9        | 0.32          |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG3  | 9        | 0.32          |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG2  | 9        | 0.32          |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG3  | 9        | 0.32          |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE1 | 16       | 0.32          |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE2 | 16       | 0.32          |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE1 | 16       | 0.32          |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE2 | 16       | 0.32          |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE1 | 17       | 0.32          |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE2 | 17       | 0.32          |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE1 | 17       | 0.32          |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE2 | 17       | 0.32          |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2  | 1        | 0.31          |
| (1,445)  | 1:81:A:VAL:HG21 | 1:95:A:LYS:HB2  | 18       | 0.31          |
| (1,445)  | 1:81:A:VAL:HG21 | 1:95:A:LYS:HB3  | 18       | 0.31          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,445)  | 1:81:A:VAL:HG22 | 1:95:A:LYS:HB2   | 18       | 0.31          |
| (1,445)  | 1:81:A:VAL:HG22 | 1:95:A:LYS:HB3   | 18       | 0.31          |
| (1,445)  | 1:81:A:VAL:HG23 | 1:95:A:LYS:HB2   | 18       | 0.31          |
| (1,445)  | 1:81:A:VAL:HG23 | 1:95:A:LYS:HB3   | 18       | 0.31          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 1        | 0.31          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1   | 19       | 0.31          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2   | 19       | 0.31          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1   | 19       | 0.31          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2   | 19       | 0.31          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1   | 19       | 0.31          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2   | 19       | 0.31          |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 3        | 0.3           |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 13       | 0.3           |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 20       | 0.3           |
| (1,954)  | 1:43:A:GLU:H    | 1:44:A:ARG:HA    | 1        | 0.3           |
| (1,954)  | 1:43:A:GLU:H    | 1:44:A:ARG:HA    | 12       | 0.3           |
| (1,954)  | 1:43:A:GLU:H    | 1:44:A:ARG:HA    | 14       | 0.3           |
| (1,903)  | 1:32:A:GLY:H    | 1:34:A:GLU:H     | 13       | 0.3           |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD2  | 7        | 0.3           |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD3  | 7        | 0.3           |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD2  | 7        | 0.3           |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD3  | 7        | 0.3           |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD2  | 7        | 0.3           |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD3  | 7        | 0.3           |
| (1,439)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HG2   | 9        | 0.3           |
| (1,439)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HG3   | 9        | 0.3           |
| (1,439)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HG2   | 9        | 0.3           |
| (1,439)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HG3   | 9        | 0.3           |
| (1,439)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HG2   | 9        | 0.3           |
| (1,439)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HG3   | 9        | 0.3           |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 19       | 0.3           |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 6        | 0.29          |
| (1,954)  | 1:43:A:GLU:H    | 1:44:A:ARG:HA    | 18       | 0.29          |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 17       | 0.29          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG12 | 5        | 0.29          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG13 | 5        | 0.29          |
| (1,1126) | 1:71:A:LEU:H    | 1:69:A:ARG:HB2   | 10       | 0.28          |
| (1,1126) | 1:71:A:LEU:H    | 1:69:A:ARG:HB2   | 11       | 0.28          |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 2        | 0.28          |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 4        | 0.28          |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 8        | 0.28          |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 15       | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1015) | 1:56:A:TYR:H     | 1:57:A:MET:HB2   | 16       | 0.28          |
| (1,954)  | 1:43:A:GLU:H     | 1:44:A:ARG:HA    | 5        | 0.28          |
| (1,903)  | 1:32:A:GLY:H     | 1:34:A:GLU:H     | 14       | 0.28          |
| (1,263)  | 1:58:A:THR:HB    | 1:60:A:TYR:HA    | 5        | 0.28          |
| (1,130)  | 1:44:A:ARG:HA    | 1:105:A:ILE:HD11 | 13       | 0.28          |
| (1,130)  | 1:44:A:ARG:HA    | 1:105:A:ILE:HD12 | 13       | 0.28          |
| (1,130)  | 1:44:A:ARG:HA    | 1:105:A:ILE:HD13 | 13       | 0.28          |
| (1,130)  | 1:44:A:ARG:HA    | 1:105:A:ILE:HD11 | 18       | 0.28          |
| (1,130)  | 1:44:A:ARG:HA    | 1:105:A:ILE:HD12 | 18       | 0.28          |
| (1,130)  | 1:44:A:ARG:HA    | 1:105:A:ILE:HD13 | 18       | 0.28          |
| (1,1313) | 1:102:A:ILE:H    | 1:101:A:LYS:HA   | 8        | 0.27          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG11  | 17       | 0.27          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG12  | 17       | 0.27          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG13  | 17       | 0.27          |
| (1,1126) | 1:71:A:LEU:H     | 1:69:A:ARG:HB2   | 1        | 0.27          |
| (1,1015) | 1:56:A:TYR:H     | 1:57:A:MET:HB2   | 9        | 0.27          |
| (1,1015) | 1:56:A:TYR:H     | 1:57:A:MET:HB2   | 11       | 0.27          |
| (1,954)  | 1:43:A:GLU:H     | 1:44:A:ARG:HA    | 2        | 0.27          |
| (1,954)  | 1:43:A:GLU:H     | 1:44:A:ARG:HA    | 13       | 0.27          |
| (1,849)  | 1:125:A:ILE:HD11 | 1:57:A:MET:HB3   | 18       | 0.27          |
| (1,849)  | 1:125:A:ILE:HD12 | 1:57:A:MET:HB3   | 18       | 0.27          |
| (1,849)  | 1:125:A:ILE:HD13 | 1:57:A:MET:HB3   | 18       | 0.27          |
| (1,792)  | 1:120:A:VAL:HA   | 1:57:A:MET:HA    | 1        | 0.27          |
| (1,792)  | 1:120:A:VAL:HA   | 1:57:A:MET:HA    | 3        | 0.27          |
| (1,792)  | 1:120:A:VAL:HA   | 1:57:A:MET:HA    | 20       | 0.27          |
| (1,334)  | 1:66:A:LEU:HD11  | 1:94:A:MET:HG2   | 2        | 0.27          |
| (1,334)  | 1:66:A:LEU:HD11  | 1:94:A:MET:HG3   | 2        | 0.27          |
| (1,334)  | 1:66:A:LEU:HD12  | 1:94:A:MET:HG2   | 2        | 0.27          |
| (1,334)  | 1:66:A:LEU:HD12  | 1:94:A:MET:HG3   | 2        | 0.27          |
| (1,334)  | 1:66:A:LEU:HD13  | 1:94:A:MET:HG2   | 2        | 0.27          |
| (1,334)  | 1:66:A:LEU:HD13  | 1:94:A:MET:HG3   | 2        | 0.27          |
| (1,121)  | 1:41:A:SER:HB3   | 1:105:A:ILE:HG12 | 3        | 0.27          |
| (1,121)  | 1:41:A:SER:HB3   | 1:105:A:ILE:HG13 | 3        | 0.27          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG11  | 11       | 0.26          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG12  | 11       | 0.26          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG13  | 11       | 0.26          |
| (1,1126) | 1:71:A:LEU:H     | 1:69:A:ARG:HB2   | 9        | 0.26          |
| (1,1126) | 1:71:A:LEU:H     | 1:69:A:ARG:HB2   | 13       | 0.26          |
| (1,1126) | 1:71:A:LEU:H     | 1:69:A:ARG:HB2   | 14       | 0.26          |
| (1,1126) | 1:71:A:LEU:H     | 1:69:A:ARG:HB2   | 16       | 0.26          |
| (1,1126) | 1:71:A:LEU:H     | 1:69:A:ARG:HB2   | 20       | 0.26          |
| (1,1015) | 1:56:A:TYR:H     | 1:57:A:MET:HB2   | 14       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,954)  | 1:43:A:GLU:H     | 1:44:A:ARG:HA    | 10       | 0.26          |
| (1,954)  | 1:43:A:GLU:H     | 1:44:A:ARG:HA    | 15       | 0.26          |
| (1,903)  | 1:32:A:GLY:H     | 1:34:A:GLU:H     | 4        | 0.26          |
| (1,804)  | 1:120:A:VAL:HG21 | 1:57:A:MET:HE1   | 11       | 0.26          |
| (1,804)  | 1:120:A:VAL:HG21 | 1:57:A:MET:HE2   | 11       | 0.26          |
| (1,804)  | 1:120:A:VAL:HG21 | 1:57:A:MET:HE3   | 11       | 0.26          |
| (1,804)  | 1:120:A:VAL:HG22 | 1:57:A:MET:HE1   | 11       | 0.26          |
| (1,804)  | 1:120:A:VAL:HG22 | 1:57:A:MET:HE2   | 11       | 0.26          |
| (1,804)  | 1:120:A:VAL:HG22 | 1:57:A:MET:HE3   | 11       | 0.26          |
| (1,804)  | 1:120:A:VAL:HG23 | 1:57:A:MET:HE1   | 11       | 0.26          |
| (1,804)  | 1:120:A:VAL:HG23 | 1:57:A:MET:HE2   | 11       | 0.26          |
| (1,804)  | 1:120:A:VAL:HG23 | 1:57:A:MET:HE3   | 11       | 0.26          |
| (1,792)  | 1:120:A:VAL:HA   | 1:57:A:MET:HA    | 2        | 0.26          |
| (1,551)  | 1:96:A:GLU:HA    | 1:99:A:ALA:HA    | 10       | 0.26          |
| (1,551)  | 1:96:A:GLU:HA    | 1:99:A:ALA:HA    | 13       | 0.26          |
| (1,132)  | 1:44:A:ARG:HD2   | 1:105:A:ILE:HD11 | 8        | 0.26          |
| (1,132)  | 1:44:A:ARG:HD2   | 1:105:A:ILE:HD12 | 8        | 0.26          |
| (1,132)  | 1:44:A:ARG:HD2   | 1:105:A:ILE:HD13 | 8        | 0.26          |
| (1,132)  | 1:44:A:ARG:HD3   | 1:105:A:ILE:HD11 | 8        | 0.26          |
| (1,132)  | 1:44:A:ARG:HD3   | 1:105:A:ILE:HD12 | 8        | 0.26          |
| (1,132)  | 1:44:A:ARG:HD3   | 1:105:A:ILE:HD13 | 8        | 0.26          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG11  | 4        | 0.25          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG12  | 4        | 0.25          |
| (1,1197) | 1:81:A:VAL:H     | 1:79:A:VAL:HG13  | 4        | 0.25          |
| (1,1126) | 1:71:A:LEU:H     | 1:69:A:ARG:HB2   | 3        | 0.25          |
| (1,1126) | 1:71:A:LEU:H     | 1:69:A:ARG:HB2   | 5        | 0.25          |
| (1,954)  | 1:43:A:GLU:H     | 1:44:A:ARG:HA    | 7        | 0.25          |
| (1,954)  | 1:43:A:GLU:H     | 1:44:A:ARG:HA    | 8        | 0.25          |
| (1,954)  | 1:43:A:GLU:H     | 1:44:A:ARG:HA    | 16       | 0.25          |
| (1,792)  | 1:120:A:VAL:HA   | 1:57:A:MET:HA    | 15       | 0.25          |
| (1,551)  | 1:96:A:GLU:HA    | 1:99:A:ALA:HA    | 9        | 0.25          |
| (1,551)  | 1:96:A:GLU:HA    | 1:99:A:ALA:HA    | 11       | 0.25          |
| (1,438)  | 1:81:A:VAL:HG11  | 1:96:A:GLU:HA    | 20       | 0.25          |
| (1,438)  | 1:81:A:VAL:HG12  | 1:96:A:GLU:HA    | 20       | 0.25          |
| (1,438)  | 1:81:A:VAL:HG13  | 1:96:A:GLU:HA    | 20       | 0.25          |
| (1,91)   | 1:38:A:ILE:HD11  | 1:64:A:ARG:HB2   | 6        | 0.25          |
| (1,91)   | 1:38:A:ILE:HD11  | 1:64:A:ARG:HB3   | 6        | 0.25          |
| (1,91)   | 1:38:A:ILE:HD12  | 1:64:A:ARG:HB2   | 6        | 0.25          |
| (1,91)   | 1:38:A:ILE:HD12  | 1:64:A:ARG:HB3   | 6        | 0.25          |
| (1,91)   | 1:38:A:ILE:HD13  | 1:64:A:ARG:HB2   | 6        | 0.25          |
| (1,91)   | 1:38:A:ILE:HD13  | 1:64:A:ARG:HB3   | 6        | 0.25          |
| (1,91)   | 1:38:A:ILE:HD11  | 1:64:A:ARG:HB2   | 8        | 0.25          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3   | 8        | 0.25          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2   | 8        | 0.25          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3   | 8        | 0.25          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2   | 8        | 0.25          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3   | 8        | 0.25          |
| (1,1126) | 1:71:A:LEU:H    | 1:69:A:ARG:HB2   | 17       | 0.24          |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 5        | 0.24          |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 7        | 0.24          |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 17       | 0.24          |
| (1,954)  | 1:43:A:GLU:H    | 1:44:A:ARG:HA    | 3        | 0.24          |
| (1,954)  | 1:43:A:GLU:H    | 1:44:A:ARG:HA    | 20       | 0.24          |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 4        | 0.24          |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 13       | 0.24          |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD11 | 2        | 0.24          |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD12 | 2        | 0.24          |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD13 | 2        | 0.24          |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD11 | 11       | 0.24          |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD12 | 11       | 0.24          |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD13 | 11       | 0.24          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 11       | 0.24          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG12 | 16       | 0.24          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG13 | 16       | 0.24          |
| (1,1126) | 1:71:A:LEU:H    | 1:69:A:ARG:HB2   | 12       | 0.23          |
| (1,1126) | 1:71:A:LEU:H    | 1:69:A:ARG:HB2   | 15       | 0.23          |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 10       | 0.23          |
| (1,930)  | 1:38:A:ILE:H    | 1:36:A:VAL:HA    | 5        | 0.23          |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 7        | 0.23          |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 10       | 0.23          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 16       | 0.23          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 20       | 0.23          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 3        | 0.23          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG12 | 14       | 0.23          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG13 | 14       | 0.23          |
| (1,117)  | 1:41:A:SER:HA   | 1:105:A:ILE:HG12 | 7        | 0.23          |
| (1,117)  | 1:41:A:SER:HA   | 1:105:A:ILE:HG13 | 7        | 0.23          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1   | 10       | 0.23          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2   | 10       | 0.23          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1   | 10       | 0.23          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2   | 10       | 0.23          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1   | 10       | 0.23          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2   | 10       | 0.23          |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA   | 2        | 0.22          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA   | 12       | 0.22          |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA   | 17       | 0.22          |
| (1,1126) | 1:71:A:LEU:H    | 1:69:A:ARG:HB2   | 2        | 0.22          |
| (1,1126) | 1:71:A:LEU:H    | 1:69:A:ARG:HB2   | 4        | 0.22          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA    | 13       | 0.22          |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 11       | 0.22          |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 12       | 0.22          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 3        | 0.22          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 7        | 0.22          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 18       | 0.22          |
| (1,117)  | 1:41:A:SER:HA   | 1:105:A:ILE:HG12 | 10       | 0.22          |
| (1,117)  | 1:41:A:SER:HA   | 1:105:A:ILE:HG13 | 10       | 0.22          |
| (1,117)  | 1:41:A:SER:HA   | 1:105:A:ILE:HG12 | 12       | 0.22          |
| (1,117)  | 1:41:A:SER:HA   | 1:105:A:ILE:HG13 | 12       | 0.22          |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE1  | 8        | 0.22          |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE2  | 8        | 0.22          |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE1  | 8        | 0.22          |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE2  | 8        | 0.22          |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE1  | 14       | 0.22          |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE2  | 14       | 0.22          |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE1  | 14       | 0.22          |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE2  | 14       | 0.22          |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA   | 15       | 0.21          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG11  | 16       | 0.21          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG12  | 16       | 0.21          |
| (1,1197) | 1:81:A:VAL:H    | 1:79:A:VAL:HG13  | 16       | 0.21          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 7        | 0.21          |
| (1,1126) | 1:71:A:LEU:H    | 1:69:A:ARG:HB2   | 18       | 0.21          |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 18       | 0.21          |
| (1,1015) | 1:56:A:TYR:H    | 1:57:A:MET:HB2   | 19       | 0.21          |
| (1,957)  | 1:44:A:ARG:H    | 1:43:A:GLU:H     | 5        | 0.21          |
| (1,954)  | 1:43:A:GLU:H    | 1:44:A:ARG:HA    | 9        | 0.21          |
| (1,903)  | 1:32:A:GLY:H    | 1:34:A:GLU:H     | 11       | 0.21          |
| (1,903)  | 1:32:A:GLY:H    | 1:34:A:GLU:H     | 17       | 0.21          |
| (1,903)  | 1:32:A:GLY:H    | 1:34:A:GLU:H     | 19       | 0.21          |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 6        | 0.21          |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD11 | 1        | 0.21          |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD12 | 1        | 0.21          |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD13 | 1        | 0.21          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 4        | 0.21          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 17       | 0.21          |
| (1,540)  | 1:94:A:MET:HE1  | 1:91:A:LEU:HA    | 17       | 0.21          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,540)  | 1:94:A:MET:HE2  | 1:91:A:LEU:HA    | 17       | 0.21          |
| (1,540)  | 1:94:A:MET:HE3  | 1:91:A:LEU:HA    | 17       | 0.21          |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD2  | 11       | 0.21          |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD3  | 11       | 0.21          |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD2  | 11       | 0.21          |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD3  | 11       | 0.21          |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD2  | 11       | 0.21          |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD3  | 11       | 0.21          |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD2  | 13       | 0.21          |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD3  | 13       | 0.21          |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD2  | 13       | 0.21          |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD3  | 13       | 0.21          |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD2  | 13       | 0.21          |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD3  | 13       | 0.21          |
| (1,439)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HG2   | 10       | 0.21          |
| (1,439)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HG3   | 10       | 0.21          |
| (1,439)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HG2   | 10       | 0.21          |
| (1,439)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HG3   | 10       | 0.21          |
| (1,439)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HG2   | 10       | 0.21          |
| (1,439)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HG3   | 10       | 0.21          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 12       | 0.21          |
| (1,141)  | 1:45:A:PRO:HG2  | 1:105:A:ILE:HD11 | 7        | 0.21          |
| (1,141)  | 1:45:A:PRO:HG2  | 1:105:A:ILE:HD12 | 7        | 0.21          |
| (1,141)  | 1:45:A:PRO:HG2  | 1:105:A:ILE:HD13 | 7        | 0.21          |
| (1,141)  | 1:45:A:PRO:HG3  | 1:105:A:ILE:HD11 | 7        | 0.21          |
| (1,141)  | 1:45:A:PRO:HG3  | 1:105:A:ILE:HD12 | 7        | 0.21          |
| (1,141)  | 1:45:A:PRO:HG3  | 1:105:A:ILE:HD13 | 7        | 0.21          |
| (1,140)  | 1:45:A:PRO:HD2  | 1:105:A:ILE:HD11 | 13       | 0.21          |
| (1,140)  | 1:45:A:PRO:HD2  | 1:105:A:ILE:HD12 | 13       | 0.21          |
| (1,140)  | 1:45:A:PRO:HD2  | 1:105:A:ILE:HD13 | 13       | 0.21          |
| (1,140)  | 1:45:A:PRO:HD3  | 1:105:A:ILE:HD11 | 13       | 0.21          |
| (1,140)  | 1:45:A:PRO:HD3  | 1:105:A:ILE:HD12 | 13       | 0.21          |
| (1,140)  | 1:45:A:PRO:HD3  | 1:105:A:ILE:HD13 | 13       | 0.21          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1   | 18       | 0.21          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2   | 18       | 0.21          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1   | 18       | 0.21          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2   | 18       | 0.21          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1   | 18       | 0.21          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2   | 18       | 0.21          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 4        | 0.2           |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 5        | 0.2           |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 16       | 0.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 8        | 0.2           |
| (1,930)  | 1:38:A:ILE:H    | 1:36:A:VAL:HA    | 3        | 0.2           |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 8        | 0.2           |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 18       | 0.2           |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 19       | 0.2           |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD11 | 3        | 0.2           |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD12 | 3        | 0.2           |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD13 | 3        | 0.2           |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD11 | 20       | 0.2           |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD12 | 20       | 0.2           |
| (1,754)  | 1:118:A:TRP:HB3 | 1:123:A:LEU:HD13 | 20       | 0.2           |
| (1,439)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HG2   | 20       | 0.2           |
| (1,439)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HG3   | 20       | 0.2           |
| (1,439)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HG2   | 20       | 0.2           |
| (1,439)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HG3   | 20       | 0.2           |
| (1,439)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HG2   | 20       | 0.2           |
| (1,439)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HG3   | 20       | 0.2           |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG2   | 13       | 0.2           |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG3   | 13       | 0.2           |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG2   | 13       | 0.2           |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG3   | 13       | 0.2           |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG2   | 13       | 0.2           |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG3   | 13       | 0.2           |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG2   | 15       | 0.2           |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG3   | 15       | 0.2           |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG2   | 15       | 0.2           |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG3   | 15       | 0.2           |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG2   | 15       | 0.2           |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG3   | 15       | 0.2           |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 2        | 0.2           |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG12 | 15       | 0.2           |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG13 | 15       | 0.2           |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE1  | 2        | 0.2           |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE2  | 2        | 0.2           |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE1  | 2        | 0.2           |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE2  | 2        | 0.2           |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB   | 10       | 0.19          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 7        | 0.19          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 14       | 0.19          |
| (1,1339) | 1:107:A:ARG:HE  | 1:108:A:ARG:H    | 20       | 0.19          |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA   | 7        | 0.19          |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA   | 16       | 0.19          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 6        | 0.19          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 19       | 0.19          |
| (1,977)  | 1:50:A:LYS:H    | 1:49:A:GLN:HG2   | 19       | 0.19          |
| (1,977)  | 1:50:A:LYS:H    | 1:49:A:GLN:HG3   | 19       | 0.19          |
| (1,930)  | 1:38:A:ILE:H    | 1:36:A:VAL:HA    | 16       | 0.19          |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 14       | 0.19          |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 16       | 0.19          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 6        | 0.19          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 7        | 0.19          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 8        | 0.19          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 14       | 0.19          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 18       | 0.19          |
| (1,439)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HG2   | 18       | 0.19          |
| (1,439)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HG3   | 18       | 0.19          |
| (1,439)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HG2   | 18       | 0.19          |
| (1,439)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HG3   | 18       | 0.19          |
| (1,439)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HG2   | 18       | 0.19          |
| (1,439)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HG3   | 18       | 0.19          |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG2   | 11       | 0.19          |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG3   | 11       | 0.19          |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG2   | 11       | 0.19          |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG3   | 11       | 0.19          |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG2   | 11       | 0.19          |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG3   | 11       | 0.19          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 6        | 0.19          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 9        | 0.19          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 17       | 0.19          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 20       | 0.19          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG12 | 13       | 0.19          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG13 | 13       | 0.19          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2   | 17       | 0.19          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3   | 17       | 0.19          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2   | 17       | 0.19          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3   | 17       | 0.19          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2   | 17       | 0.19          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3   | 17       | 0.19          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2   | 20       | 0.19          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3   | 20       | 0.19          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2   | 20       | 0.19          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3   | 20       | 0.19          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2   | 20       | 0.19          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3   | 20       | 0.19          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE1  | 3        | 0.19          |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE2  | 3        | 0.19          |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE1  | 3        | 0.19          |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE2  | 3        | 0.19          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE1   | 9        | 0.19          |
| (1,52)   | 1:36:A:VAL:HG11 | 1:60:A:TYR:HE2   | 9        | 0.19          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE1   | 9        | 0.19          |
| (1,52)   | 1:36:A:VAL:HG12 | 1:60:A:TYR:HE2   | 9        | 0.19          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE1   | 9        | 0.19          |
| (1,52)   | 1:36:A:VAL:HG13 | 1:60:A:TYR:HE2   | 9        | 0.19          |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB   | 6        | 0.18          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 3        | 0.18          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 10       | 0.18          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 12       | 0.18          |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA   | 10       | 0.18          |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA   | 18       | 0.18          |
| (1,957)  | 1:44:A:ARG:H    | 1:43:A:GLU:H     | 2        | 0.18          |
| (1,918)  | 1:36:A:VAL:H    | 1:35:A:ASN:HB2   | 11       | 0.18          |
| (1,792)  | 1:120:A:VAL:HA  | 1:57:A:MET:HA    | 9        | 0.18          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 5        | 0.18          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 15       | 0.18          |
| (1,445)  | 1:81:A:VAL:HG21 | 1:95:A:LYS:HB2   | 7        | 0.18          |
| (1,445)  | 1:81:A:VAL:HG21 | 1:95:A:LYS:HB3   | 7        | 0.18          |
| (1,445)  | 1:81:A:VAL:HG22 | 1:95:A:LYS:HB2   | 7        | 0.18          |
| (1,445)  | 1:81:A:VAL:HG22 | 1:95:A:LYS:HB3   | 7        | 0.18          |
| (1,445)  | 1:81:A:VAL:HG23 | 1:95:A:LYS:HB2   | 7        | 0.18          |
| (1,445)  | 1:81:A:VAL:HG23 | 1:95:A:LYS:HB3   | 7        | 0.18          |
| (1,439)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HG2   | 13       | 0.18          |
| (1,439)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HG3   | 13       | 0.18          |
| (1,439)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HG2   | 13       | 0.18          |
| (1,439)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HG3   | 13       | 0.18          |
| (1,439)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HG2   | 13       | 0.18          |
| (1,439)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HG3   | 13       | 0.18          |
| (1,381)  | 1:73:A:ILE:HB   | 1:89:A:PRO:HB2   | 6        | 0.18          |
| (1,381)  | 1:73:A:ILE:HB   | 1:89:A:PRO:HB3   | 6        | 0.18          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA    | 9        | 0.18          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA    | 15       | 0.18          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA    | 16       | 0.18          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 15       | 0.18          |
| (1,135)  | 1:44:A:ARG:HG2  | 1:105:A:ILE:HD11 | 13       | 0.18          |
| (1,135)  | 1:44:A:ARG:HG2  | 1:105:A:ILE:HD12 | 13       | 0.18          |
| (1,135)  | 1:44:A:ARG:HG2  | 1:105:A:ILE:HD13 | 13       | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,135)  | 1:44:A:ARG:HG3   | 1:105:A:ILE:HD11 | 13       | 0.18          |
| (1,135)  | 1:44:A:ARG:HG3   | 1:105:A:ILE:HD12 | 13       | 0.18          |
| (1,135)  | 1:44:A:ARG:HG3   | 1:105:A:ILE:HD13 | 13       | 0.18          |
| (1,116)  | 1:41:A:SER:HA    | 1:105:A:ILE:HD11 | 2        | 0.18          |
| (1,116)  | 1:41:A:SER:HA    | 1:105:A:ILE:HD12 | 2        | 0.18          |
| (1,116)  | 1:41:A:SER:HA    | 1:105:A:ILE:HD13 | 2        | 0.18          |
| (1,91)   | 1:38:A:ILE:HD11  | 1:64:A:ARG:HB2   | 16       | 0.18          |
| (1,91)   | 1:38:A:ILE:HD11  | 1:64:A:ARG:HB3   | 16       | 0.18          |
| (1,91)   | 1:38:A:ILE:HD12  | 1:64:A:ARG:HB2   | 16       | 0.18          |
| (1,91)   | 1:38:A:ILE:HD12  | 1:64:A:ARG:HB3   | 16       | 0.18          |
| (1,91)   | 1:38:A:ILE:HD13  | 1:64:A:ARG:HB2   | 16       | 0.18          |
| (1,91)   | 1:38:A:ILE:HD13  | 1:64:A:ARG:HB3   | 16       | 0.18          |
| (1,1731) | 1:52:A:ILE:H     | 1:52:A:ILE:HG12  | 19       | 0.17          |
| (1,1731) | 1:52:A:ILE:H     | 1:52:A:ILE:HG13  | 19       | 0.17          |
| (1,1374) | 1:110:A:LEU:H    | 1:114:A:SER:HB3  | 1        | 0.17          |
| (1,1374) | 1:110:A:LEU:H    | 1:114:A:SER:HB3  | 6        | 0.17          |
| (1,1374) | 1:110:A:LEU:H    | 1:114:A:SER:HB3  | 15       | 0.17          |
| (1,1339) | 1:107:A:ARG:HE   | 1:108:A:ARG:H    | 12       | 0.17          |
| (1,1135) | 1:72:A:GLN:H     | 1:69:A:ARG:HB2   | 4        | 0.17          |
| (1,1066) | 1:63:A:ALA:H     | 1:61:A:GLU:HB2   | 10       | 0.17          |
| (1,930)  | 1:38:A:ILE:H     | 1:36:A:VAL:HA    | 20       | 0.17          |
| (1,903)  | 1:32:A:GLY:H     | 1:34:A:GLU:H     | 16       | 0.17          |
| (1,898)  | 1:30:A:GLU:H     | 1:29:A:GLU:HA    | 18       | 0.17          |
| (1,891)  | 1:27:A:ASN:H     | 1:26:A:GLU:HA    | 3        | 0.17          |
| (1,849)  | 1:125:A:ILE:HD11 | 1:57:A:MET:HB3   | 2        | 0.17          |
| (1,849)  | 1:125:A:ILE:HD12 | 1:57:A:MET:HB3   | 2        | 0.17          |
| (1,849)  | 1:125:A:ILE:HD13 | 1:57:A:MET:HB3   | 2        | 0.17          |
| (1,754)  | 1:118:A:TRP:HB3  | 1:123:A:LEU:HD11 | 12       | 0.17          |
| (1,754)  | 1:118:A:TRP:HB3  | 1:123:A:LEU:HD12 | 12       | 0.17          |
| (1,754)  | 1:118:A:TRP:HB3  | 1:123:A:LEU:HD13 | 12       | 0.17          |
| (1,478)  | 1:87:A:THR:HB    | 1:83:A:LEU:HG    | 18       | 0.17          |
| (1,450)  | 1:81:A:VAL:HG21  | 1:96:A:GLU:HG2   | 3        | 0.17          |
| (1,450)  | 1:81:A:VAL:HG21  | 1:96:A:GLU:HG3   | 3        | 0.17          |
| (1,450)  | 1:81:A:VAL:HG22  | 1:96:A:GLU:HG2   | 3        | 0.17          |
| (1,450)  | 1:81:A:VAL:HG22  | 1:96:A:GLU:HG3   | 3        | 0.17          |
| (1,450)  | 1:81:A:VAL:HG23  | 1:96:A:GLU:HG2   | 3        | 0.17          |
| (1,450)  | 1:81:A:VAL:HG23  | 1:96:A:GLU:HG3   | 3        | 0.17          |
| (1,426)  | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG21  | 7        | 0.17          |
| (1,426)  | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG22  | 7        | 0.17          |
| (1,426)  | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG23  | 7        | 0.17          |
| (1,426)  | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG21  | 7        | 0.17          |
| (1,426)  | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG22  | 7        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,426)  | 1:79:A:VAL:HG22 | 1:92:A:ILE:HG23 | 7        | 0.17          |
| (1,426)  | 1:79:A:VAL:HG23 | 1:92:A:ILE:HG21 | 7        | 0.17          |
| (1,426)  | 1:79:A:VAL:HG23 | 1:92:A:ILE:HG22 | 7        | 0.17          |
| (1,426)  | 1:79:A:VAL:HG23 | 1:92:A:ILE:HG23 | 7        | 0.17          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA   | 4        | 0.17          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA   | 10       | 0.17          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA   | 12       | 0.17          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA   | 14       | 0.17          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA   | 18       | 0.17          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA   | 19       | 0.17          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA   | 10       | 0.17          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2  | 3        | 0.17          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3  | 3        | 0.17          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2  | 3        | 0.17          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3  | 3        | 0.17          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2  | 3        | 0.17          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3  | 3        | 0.17          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2  | 13       | 0.17          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3  | 13       | 0.17          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2  | 13       | 0.17          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3  | 13       | 0.17          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2  | 13       | 0.17          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3  | 13       | 0.17          |
| (1,1731) | 1:52:A:ILE:H    | 1:52:A:ILE:HG12 | 14       | 0.16          |
| (1,1731) | 1:52:A:ILE:H    | 1:52:A:ILE:HG13 | 14       | 0.16          |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB  | 2        | 0.16          |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB  | 7        | 0.16          |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB  | 18       | 0.16          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3 | 11       | 0.16          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3 | 13       | 0.16          |
| (1,1339) | 1:107:A:ARG:HE  | 1:108:A:ARG:H   | 4        | 0.16          |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA  | 6        | 0.16          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2  | 15       | 0.16          |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA   | 7        | 0.16          |
| (1,973)  | 1:49:A:GLN:H    | 1:48:A:ASN:HA   | 16       | 0.16          |
| (1,957)  | 1:44:A:ARG:H    | 1:43:A:GLU:H    | 7        | 0.16          |
| (1,918)  | 1:36:A:VAL:H    | 1:35:A:ASN:HB2  | 19       | 0.16          |
| (1,903)  | 1:32:A:GLY:H    | 1:34:A:GLU:H    | 9        | 0.16          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA   | 2        | 0.16          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA   | 19       | 0.16          |
| (1,478)  | 1:87:A:THR:HB   | 1:83:A:LEU:HG   | 4        | 0.16          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA   | 3        | 0.16          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA    | 8        | 0.16          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA    | 13       | 0.16          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA    | 17       | 0.16          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA    | 20       | 0.16          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 8        | 0.16          |
| (1,206)  | 1:55:A:PRO:HB2  | 1:118:A:TRP:HZ3  | 17       | 0.16          |
| (1,206)  | 1:55:A:PRO:HB3  | 1:118:A:TRP:HZ3  | 17       | 0.16          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG12 | 19       | 0.16          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG13 | 19       | 0.16          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2   | 2        | 0.16          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3   | 2        | 0.16          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2   | 2        | 0.16          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3   | 2        | 0.16          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2   | 2        | 0.16          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3   | 2        | 0.16          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 9        | 0.15          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 17       | 0.15          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 18       | 0.15          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 19       | 0.15          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 20       | 0.15          |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA   | 3        | 0.15          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 5        | 0.15          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 12       | 0.15          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 14       | 0.15          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 16       | 0.15          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 18       | 0.15          |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA    | 6        | 0.15          |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA    | 8        | 0.15          |
| (1,957)  | 1:44:A:ARG:H    | 1:43:A:GLU:H     | 9        | 0.15          |
| (1,957)  | 1:44:A:ARG:H    | 1:43:A:GLU:H     | 12       | 0.15          |
| (1,957)  | 1:44:A:ARG:H    | 1:43:A:GLU:H     | 20       | 0.15          |
| (1,930)  | 1:38:A:ILE:H    | 1:36:A:VAL:HA    | 1        | 0.15          |
| (1,930)  | 1:38:A:ILE:H    | 1:36:A:VAL:HA    | 4        | 0.15          |
| (1,903)  | 1:32:A:GLY:H    | 1:34:A:GLU:H     | 15       | 0.15          |
| (1,892)  | 1:27:A:ASN:H    | 1:26:A:GLU:HB2   | 14       | 0.15          |
| (1,892)  | 1:27:A:ASN:H    | 1:26:A:GLU:HB3   | 14       | 0.15          |
| (1,891)  | 1:27:A:ASN:H    | 1:26:A:GLU:HA    | 14       | 0.15          |
| (1,884)  | 1:21:A:GLY:H    | 1:22:A:LEU:H     | 3        | 0.15          |
| (1,783)  | 1:118:A:TRP:HZ3 | 1:122:A:GLU:HA   | 6        | 0.15          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 1        | 0.15          |
| (1,551)  | 1:96:A:GLU:HA   | 1:99:A:ALA:HA    | 12       | 0.15          |
| (1,478)  | 1:87:A:THR:HB   | 1:83:A:LEU:HG    | 10       | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,478)  | 1:87:A:THR:HB   | 1:83:A:LEU:HG    | 16       | 0.15          |
| (1,478)  | 1:87:A:THR:HB   | 1:83:A:LEU:HG    | 20       | 0.15          |
| (1,438)  | 1:81:A:VAL:HG11 | 1:96:A:GLU:HA    | 4        | 0.15          |
| (1,438)  | 1:81:A:VAL:HG12 | 1:96:A:GLU:HA    | 4        | 0.15          |
| (1,438)  | 1:81:A:VAL:HG13 | 1:96:A:GLU:HA    | 4        | 0.15          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA    | 2        | 0.15          |
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA    | 6        | 0.15          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA    | 4        | 0.15          |
| (1,254)  | 1:57:A:MET:HG2  | 1:61:A:GLU:HB3   | 6        | 0.15          |
| (1,254)  | 1:57:A:MET:HG3  | 1:61:A:GLU:HB3   | 6        | 0.15          |
| (1,130)  | 1:44:A:ARG:HA   | 1:105:A:ILE:HD11 | 16       | 0.15          |
| (1,130)  | 1:44:A:ARG:HA   | 1:105:A:ILE:HD12 | 16       | 0.15          |
| (1,130)  | 1:44:A:ARG:HA   | 1:105:A:ILE:HD13 | 16       | 0.15          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG12 | 11       | 0.15          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG13 | 11       | 0.15          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG12 | 17       | 0.15          |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG13 | 17       | 0.15          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2   | 15       | 0.15          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3   | 15       | 0.15          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2   | 15       | 0.15          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3   | 15       | 0.15          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2   | 15       | 0.15          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3   | 15       | 0.15          |
| (1,1731) | 1:52:A:ILE:H    | 1:52:A:ILE:HG12  | 9        | 0.14          |
| (1,1731) | 1:52:A:ILE:H    | 1:52:A:ILE:HG13  | 9        | 0.14          |
| (1,1731) | 1:52:A:ILE:H    | 1:52:A:ILE:HG12  | 17       | 0.14          |
| (1,1731) | 1:52:A:ILE:H    | 1:52:A:ILE:HG13  | 17       | 0.14          |
| (1,1534) | 1:57:A:MET:H    | 1:57:A:MET:HB2   | 5        | 0.14          |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB   | 8        | 0.14          |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB   | 9        | 0.14          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 2        | 0.14          |
| (1,1374) | 1:110:A:LEU:H   | 1:114:A:SER:HB3  | 8        | 0.14          |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA   | 1        | 0.14          |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA   | 14       | 0.14          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 2        | 0.14          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 3        | 0.14          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 17       | 0.14          |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA    | 19       | 0.14          |
| (1,1017) | 1:56:A:TYR:H    | 1:108:A:ARG:HE   | 12       | 0.14          |
| (1,998)  | 1:53:A:THR:H    | 1:118:A:TRP:HH2  | 2        | 0.14          |
| (1,957)  | 1:44:A:ARG:H    | 1:43:A:GLU:H     | 3        | 0.14          |
| (1,955)  | 1:44:A:ARG:H    | 1:43:A:GLU:HA    | 4        | 0.14          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,930) | 1:38:A:ILE:H     | 1:36:A:VAL:HA   | 6        | 0.14          |
| (1,911) | 1:35:A:ASN:H     | 1:34:A:GLU:HB3  | 3        | 0.14          |
| (1,903) | 1:32:A:GLY:H     | 1:34:A:GLU:H    | 12       | 0.14          |
| (1,898) | 1:30:A:GLU:H     | 1:29:A:GLU:HA   | 20       | 0.14          |
| (1,870) | 1:13:A:PHE:H     | 1:12:A:ASP:HA   | 10       | 0.14          |
| (1,804) | 1:120:A:VAL:HG21 | 1:57:A:MET:HE1  | 3        | 0.14          |
| (1,804) | 1:120:A:VAL:HG21 | 1:57:A:MET:HE2  | 3        | 0.14          |
| (1,804) | 1:120:A:VAL:HG21 | 1:57:A:MET:HE3  | 3        | 0.14          |
| (1,804) | 1:120:A:VAL:HG22 | 1:57:A:MET:HE1  | 3        | 0.14          |
| (1,804) | 1:120:A:VAL:HG22 | 1:57:A:MET:HE2  | 3        | 0.14          |
| (1,804) | 1:120:A:VAL:HG22 | 1:57:A:MET:HE3  | 3        | 0.14          |
| (1,804) | 1:120:A:VAL:HG23 | 1:57:A:MET:HE1  | 3        | 0.14          |
| (1,804) | 1:120:A:VAL:HG23 | 1:57:A:MET:HE2  | 3        | 0.14          |
| (1,804) | 1:120:A:VAL:HG23 | 1:57:A:MET:HE3  | 3        | 0.14          |
| (1,478) | 1:87:A:THR:HB    | 1:83:A:LEU:HG   | 7        | 0.14          |
| (1,478) | 1:87:A:THR:HB    | 1:83:A:LEU:HG   | 13       | 0.14          |
| (1,439) | 1:81:A:VAL:HG11  | 1:96:A:GLU:HG2  | 11       | 0.14          |
| (1,439) | 1:81:A:VAL:HG11  | 1:96:A:GLU:HG3  | 11       | 0.14          |
| (1,439) | 1:81:A:VAL:HG12  | 1:96:A:GLU:HG2  | 11       | 0.14          |
| (1,439) | 1:81:A:VAL:HG12  | 1:96:A:GLU:HG3  | 11       | 0.14          |
| (1,439) | 1:81:A:VAL:HG13  | 1:96:A:GLU:HG2  | 11       | 0.14          |
| (1,439) | 1:81:A:VAL:HG13  | 1:96:A:GLU:HG3  | 11       | 0.14          |
| (1,426) | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG21 | 15       | 0.14          |
| (1,426) | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG22 | 15       | 0.14          |
| (1,426) | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG23 | 15       | 0.14          |
| (1,426) | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG21 | 15       | 0.14          |
| (1,426) | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG22 | 15       | 0.14          |
| (1,426) | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG23 | 15       | 0.14          |
| (1,426) | 1:79:A:VAL:HG23  | 1:92:A:ILE:HG21 | 15       | 0.14          |
| (1,426) | 1:79:A:VAL:HG23  | 1:92:A:ILE:HG22 | 15       | 0.14          |
| (1,426) | 1:79:A:VAL:HG23  | 1:92:A:ILE:HG23 | 15       | 0.14          |
| (1,426) | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG21 | 18       | 0.14          |
| (1,426) | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG22 | 18       | 0.14          |
| (1,426) | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG23 | 18       | 0.14          |
| (1,426) | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG21 | 18       | 0.14          |
| (1,426) | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG22 | 18       | 0.14          |
| (1,426) | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG23 | 18       | 0.14          |
| (1,426) | 1:79:A:VAL:HG23  | 1:92:A:ILE:HG21 | 18       | 0.14          |
| (1,426) | 1:79:A:VAL:HG23  | 1:92:A:ILE:HG22 | 18       | 0.14          |
| (1,426) | 1:79:A:VAL:HG23  | 1:92:A:ILE:HG23 | 18       | 0.14          |
| (1,341) | 1:68:A:THR:HA    | 1:65:A:VAL:HA   | 5        | 0.14          |
| (1,341) | 1:68:A:THR:HA    | 1:65:A:VAL:HA   | 7        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,341)  | 1:68:A:THR:HA   | 1:65:A:VAL:HA   | 11       | 0.14          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2  | 4        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3  | 4        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2  | 4        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3  | 4        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2  | 4        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3  | 4        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2  | 7        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3  | 7        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2  | 7        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3  | 7        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2  | 7        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3  | 7        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2  | 9        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3  | 9        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2  | 9        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3  | 9        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2  | 9        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3  | 9        | 0.14          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2  | 11       | 0.14          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3  | 11       | 0.14          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2  | 11       | 0.14          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3  | 11       | 0.14          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2  | 11       | 0.14          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3  | 11       | 0.14          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2  | 12       | 0.14          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3  | 12       | 0.14          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2  | 12       | 0.14          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3  | 12       | 0.14          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2  | 12       | 0.14          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3  | 12       | 0.14          |
| (1,1731) | 1:52:A:ILE:H    | 1:52:A:ILE:HG12 | 7        | 0.13          |
| (1,1731) | 1:52:A:ILE:H    | 1:52:A:ILE:HG13 | 7        | 0.13          |
| (1,1534) | 1:57:A:MET:H    | 1:57:A:MET:HB2  | 4        | 0.13          |
| (1,1534) | 1:57:A:MET:H    | 1:57:A:MET:HB2  | 14       | 0.13          |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB  | 15       | 0.13          |
| (1,1492) | 1:124:A:ILE:H   | 1:123:A:LEU:HG  | 14       | 0.13          |
| (1,1339) | 1:107:A:ARG:HE  | 1:108:A:ARG:H   | 15       | 0.13          |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA  | 20       | 0.13          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2  | 1        | 0.13          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2  | 9        | 0.13          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2  | 11       | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1126) | 1:71:A:LEU:H     | 1:69:A:ARG:HB2  | 7        | 0.13          |
| (1,1071) | 1:63:A:ALA:H     | 1:65:A:VAL:HB   | 6        | 0.13          |
| (1,1066) | 1:63:A:ALA:H     | 1:61:A:GLU:HB2  | 7        | 0.13          |
| (1,1066) | 1:63:A:ALA:H     | 1:61:A:GLU:HB2  | 12       | 0.13          |
| (1,957)  | 1:44:A:ARG:H     | 1:43:A:GLU:H    | 1        | 0.13          |
| (1,957)  | 1:44:A:ARG:H     | 1:43:A:GLU:H    | 10       | 0.13          |
| (1,957)  | 1:44:A:ARG:H     | 1:43:A:GLU:H    | 11       | 0.13          |
| (1,957)  | 1:44:A:ARG:H     | 1:43:A:GLU:H    | 16       | 0.13          |
| (1,957)  | 1:44:A:ARG:H     | 1:43:A:GLU:H    | 19       | 0.13          |
| (1,902)  | 1:32:A:GLY:H     | 1:33:A:GLN:H    | 13       | 0.13          |
| (1,893)  | 1:28:A:ALA:H     | 1:27:A:ASN:HA   | 12       | 0.13          |
| (1,870)  | 1:13:A:PHE:H     | 1:12:A:ASP:HA   | 7        | 0.13          |
| (1,804)  | 1:120:A:VAL:HG21 | 1:57:A:MET:HE1  | 2        | 0.13          |
| (1,804)  | 1:120:A:VAL:HG21 | 1:57:A:MET:HE2  | 2        | 0.13          |
| (1,804)  | 1:120:A:VAL:HG21 | 1:57:A:MET:HE3  | 2        | 0.13          |
| (1,804)  | 1:120:A:VAL:HG22 | 1:57:A:MET:HE1  | 2        | 0.13          |
| (1,804)  | 1:120:A:VAL:HG22 | 1:57:A:MET:HE2  | 2        | 0.13          |
| (1,804)  | 1:120:A:VAL:HG22 | 1:57:A:MET:HE3  | 2        | 0.13          |
| (1,804)  | 1:120:A:VAL:HG23 | 1:57:A:MET:HE1  | 2        | 0.13          |
| (1,804)  | 1:120:A:VAL:HG23 | 1:57:A:MET:HE2  | 2        | 0.13          |
| (1,804)  | 1:120:A:VAL:HG23 | 1:57:A:MET:HE3  | 2        | 0.13          |
| (1,748)  | 1:118:A:TRP:HA   | 1:106:A:ILE:HB  | 14       | 0.13          |
| (1,678)  | 1:109:A:TYR:HB2  | 1:115:A:TYR:HA  | 1        | 0.13          |
| (1,478)  | 1:87:A:THR:HB    | 1:83:A:LEU:HG   | 11       | 0.13          |
| (1,478)  | 1:87:A:THR:HB    | 1:83:A:LEU:HG   | 17       | 0.13          |
| (1,426)  | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG21 | 5        | 0.13          |
| (1,426)  | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG22 | 5        | 0.13          |
| (1,426)  | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG23 | 5        | 0.13          |
| (1,426)  | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG21 | 5        | 0.13          |
| (1,426)  | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG22 | 5        | 0.13          |
| (1,426)  | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG23 | 5        | 0.13          |
| (1,426)  | 1:79:A:VAL:HG23  | 1:92:A:ILE:HG21 | 5        | 0.13          |
| (1,426)  | 1:79:A:VAL:HG23  | 1:92:A:ILE:HG22 | 5        | 0.13          |
| (1,426)  | 1:79:A:VAL:HG23  | 1:92:A:ILE:HG23 | 5        | 0.13          |
| (1,341)  | 1:68:A:THR:HA    | 1:65:A:VAL:HA   | 1        | 0.13          |
| (1,206)  | 1:55:A:PRO:HB2   | 1:118:A:TRP:HZ3 | 1        | 0.13          |
| (1,206)  | 1:55:A:PRO:HB3   | 1:118:A:TRP:HZ3 | 1        | 0.13          |
| (1,206)  | 1:55:A:PRO:HB2   | 1:118:A:TRP:HZ3 | 9        | 0.13          |
| (1,206)  | 1:55:A:PRO:HB3   | 1:118:A:TRP:HZ3 | 9        | 0.13          |
| (1,199)  | 1:55:A:PRO:HA    | 1:118:A:TRP:HZ2 | 9        | 0.13          |
| (1,91)   | 1:38:A:ILE:HD11  | 1:64:A:ARG:HB2  | 14       | 0.13          |
| (1,91)   | 1:38:A:ILE:HD11  | 1:64:A:ARG:HB3  | 14       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2  | 14       | 0.13          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3  | 14       | 0.13          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2  | 14       | 0.13          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3  | 14       | 0.13          |
| (2,27)   | 1:68:A:THR:O    | 1:72:A:GLN:H    | 11       | 0.12          |
| (2,27)   | 1:68:A:THR:O    | 1:72:A:GLN:H    | 14       | 0.12          |
| (1,1534) | 1:57:A:MET:H    | 1:57:A:MET:HB2  | 19       | 0.12          |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB  | 14       | 0.12          |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB  | 17       | 0.12          |
| (1,1492) | 1:124:A:ILE:H   | 1:123:A:LEU:HG  | 8        | 0.12          |
| (1,1407) | 1:116:A:GLU:H   | 1:107:A:ARG:HE  | 13       | 0.12          |
| (1,1339) | 1:107:A:ARG:HE  | 1:108:A:ARG:H   | 7        | 0.12          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2  | 13       | 0.12          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2  | 20       | 0.12          |
| (1,1126) | 1:71:A:LEU:H    | 1:69:A:ARG:HB2  | 6        | 0.12          |
| (1,1126) | 1:71:A:LEU:H    | 1:69:A:ARG:HB2  | 8        | 0.12          |
| (1,1126) | 1:71:A:LEU:H    | 1:69:A:ARG:HB2  | 19       | 0.12          |
| (1,1071) | 1:63:A:ALA:H    | 1:65:A:VAL:HB   | 4        | 0.12          |
| (1,1071) | 1:63:A:ALA:H    | 1:65:A:VAL:HB   | 7        | 0.12          |
| (1,1071) | 1:63:A:ALA:H    | 1:65:A:VAL:HB   | 11       | 0.12          |
| (1,1071) | 1:63:A:ALA:H    | 1:65:A:VAL:HB   | 13       | 0.12          |
| (1,1071) | 1:63:A:ALA:H    | 1:65:A:VAL:HB   | 17       | 0.12          |
| (1,1066) | 1:63:A:ALA:H    | 1:61:A:GLU:HB2  | 2        | 0.12          |
| (1,1066) | 1:63:A:ALA:H    | 1:61:A:GLU:HB2  | 6        | 0.12          |
| (1,1066) | 1:63:A:ALA:H    | 1:61:A:GLU:HB2  | 8        | 0.12          |
| (1,1066) | 1:63:A:ALA:H    | 1:61:A:GLU:HB2  | 15       | 0.12          |
| (1,1066) | 1:63:A:ALA:H    | 1:61:A:GLU:HB2  | 18       | 0.12          |
| (1,998)  | 1:53:A:THR:H    | 1:118:A:TRP:HH2 | 5        | 0.12          |
| (1,978)  | 1:51:A:ARG:HE   | 1:118:A:TRP:HH2 | 11       | 0.12          |
| (1,957)  | 1:44:A:ARG:H    | 1:43:A:GLU:H    | 14       | 0.12          |
| (1,957)  | 1:44:A:ARG:H    | 1:43:A:GLU:H    | 15       | 0.12          |
| (1,957)  | 1:44:A:ARG:H    | 1:43:A:GLU:H    | 18       | 0.12          |
| (1,891)  | 1:27:A:ASN:H    | 1:26:A:GLU:HA   | 7        | 0.12          |
| (1,608)  | 1:105:A:ILE:HB  | 1:117:A:ASP:HA  | 5        | 0.12          |
| (1,608)  | 1:105:A:ILE:HB  | 1:117:A:ASP:HA  | 19       | 0.12          |
| (1,478)  | 1:87:A:THR:HB   | 1:83:A:LEU:HG   | 6        | 0.12          |
| (1,426)  | 1:79:A:VAL:HG21 | 1:92:A:ILE:HG21 | 20       | 0.12          |
| (1,426)  | 1:79:A:VAL:HG21 | 1:92:A:ILE:HG22 | 20       | 0.12          |
| (1,426)  | 1:79:A:VAL:HG21 | 1:92:A:ILE:HG23 | 20       | 0.12          |
| (1,426)  | 1:79:A:VAL:HG22 | 1:92:A:ILE:HG21 | 20       | 0.12          |
| (1,426)  | 1:79:A:VAL:HG22 | 1:92:A:ILE:HG22 | 20       | 0.12          |
| (1,426)  | 1:79:A:VAL:HG22 | 1:92:A:ILE:HG23 | 20       | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,426)  | 1:79:A:VAL:HG23 | 1:92:A:ILE:HG21  | 20       | 0.12          |
| (1,426)  | 1:79:A:VAL:HG23 | 1:92:A:ILE:HG22  | 20       | 0.12          |
| (1,426)  | 1:79:A:VAL:HG23 | 1:92:A:ILE:HG23  | 20       | 0.12          |
| (1,206)  | 1:55:A:PRO:HB2  | 1:118:A:TRP:HZ3  | 18       | 0.12          |
| (1,206)  | 1:55:A:PRO:HB3  | 1:118:A:TRP:HZ3  | 18       | 0.12          |
| (1,130)  | 1:44:A:ARG:HA   | 1:105:A:ILE:HD11 | 6        | 0.12          |
| (1,130)  | 1:44:A:ARG:HA   | 1:105:A:ILE:HD12 | 6        | 0.12          |
| (1,130)  | 1:44:A:ARG:HA   | 1:105:A:ILE:HD13 | 6        | 0.12          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2   | 1        | 0.12          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3   | 1        | 0.12          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2   | 1        | 0.12          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3   | 1        | 0.12          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2   | 1        | 0.12          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3   | 1        | 0.12          |
| (1,1534) | 1:57:A:MET:H    | 1:57:A:MET:HB2   | 10       | 0.11          |
| (1,1534) | 1:57:A:MET:H    | 1:57:A:MET:HB2   | 11       | 0.11          |
| (1,1534) | 1:57:A:MET:H    | 1:57:A:MET:HB2   | 17       | 0.11          |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB   | 11       | 0.11          |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB   | 16       | 0.11          |
| (1,1492) | 1:124:A:ILE:H   | 1:123:A:LEU:HG   | 1        | 0.11          |
| (1,1492) | 1:124:A:ILE:H   | 1:123:A:LEU:HG   | 3        | 0.11          |
| (1,1492) | 1:124:A:ILE:H   | 1:123:A:LEU:HG   | 6        | 0.11          |
| (1,1492) | 1:124:A:ILE:H   | 1:123:A:LEU:HG   | 10       | 0.11          |
| (1,1492) | 1:124:A:ILE:H   | 1:123:A:LEU:HG   | 15       | 0.11          |
| (1,1492) | 1:124:A:ILE:H   | 1:123:A:LEU:HG   | 17       | 0.11          |
| (1,1237) | 1:88:A:ASP:H    | 1:92:A:ILE:HB    | 14       | 0.11          |
| (1,1135) | 1:72:A:GLN:H    | 1:69:A:ARG:HB2   | 10       | 0.11          |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA    | 3        | 0.11          |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA    | 4        | 0.11          |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA    | 9        | 0.11          |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA    | 17       | 0.11          |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA    | 18       | 0.11          |
| (1,1071) | 1:63:A:ALA:H    | 1:65:A:VAL:HB    | 2        | 0.11          |
| (1,1071) | 1:63:A:ALA:H    | 1:65:A:VAL:HB    | 5        | 0.11          |
| (1,1071) | 1:63:A:ALA:H    | 1:65:A:VAL:HB    | 8        | 0.11          |
| (1,1071) | 1:63:A:ALA:H    | 1:65:A:VAL:HB    | 10       | 0.11          |
| (1,1071) | 1:63:A:ALA:H    | 1:65:A:VAL:HB    | 15       | 0.11          |
| (1,1066) | 1:63:A:ALA:H    | 1:61:A:GLU:HB2   | 1        | 0.11          |
| (1,1066) | 1:63:A:ALA:H    | 1:61:A:GLU:HB2   | 17       | 0.11          |
| (1,998)  | 1:53:A:THR:H    | 1:118:A:TRP:HH2  | 16       | 0.11          |
| (1,978)  | 1:51:A:ARG:HE   | 1:118:A:TRP:HH2  | 4        | 0.11          |
| (1,957)  | 1:44:A:ARG:H    | 1:43:A:GLU:H     | 6        | 0.11          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,930) | 1:38:A:ILE:H     | 1:36:A:VAL:HA   | 2        | 0.11          |
| (1,930) | 1:38:A:ILE:H     | 1:36:A:VAL:HA   | 15       | 0.11          |
| (1,918) | 1:36:A:VAL:H     | 1:35:A:ASN:HB2  | 6        | 0.11          |
| (1,903) | 1:32:A:GLY:H     | 1:34:A:GLU:H    | 20       | 0.11          |
| (1,804) | 1:120:A:VAL:HG21 | 1:57:A:MET:HE1  | 8        | 0.11          |
| (1,804) | 1:120:A:VAL:HG21 | 1:57:A:MET:HE2  | 8        | 0.11          |
| (1,804) | 1:120:A:VAL:HG21 | 1:57:A:MET:HE3  | 8        | 0.11          |
| (1,804) | 1:120:A:VAL:HG22 | 1:57:A:MET:HE1  | 8        | 0.11          |
| (1,804) | 1:120:A:VAL:HG22 | 1:57:A:MET:HE2  | 8        | 0.11          |
| (1,804) | 1:120:A:VAL:HG22 | 1:57:A:MET:HE3  | 8        | 0.11          |
| (1,804) | 1:120:A:VAL:HG23 | 1:57:A:MET:HE1  | 8        | 0.11          |
| (1,804) | 1:120:A:VAL:HG23 | 1:57:A:MET:HE2  | 8        | 0.11          |
| (1,804) | 1:120:A:VAL:HG23 | 1:57:A:MET:HE3  | 8        | 0.11          |
| (1,783) | 1:118:A:TRP:HZ3  | 1:122:A:GLU:HA  | 11       | 0.11          |
| (1,748) | 1:118:A:TRP:HA   | 1:106:A:ILE:HB  | 4        | 0.11          |
| (1,669) | 1:108:A:ARG:HG2  | 1:118:A:TRP:HD1 | 6        | 0.11          |
| (1,669) | 1:108:A:ARG:HG3  | 1:118:A:TRP:HD1 | 6        | 0.11          |
| (1,629) | 1:106:A:ILE:HD11 | 1:57:A:MET:HE1  | 12       | 0.11          |
| (1,629) | 1:106:A:ILE:HD11 | 1:57:A:MET:HE2  | 12       | 0.11          |
| (1,629) | 1:106:A:ILE:HD11 | 1:57:A:MET:HE3  | 12       | 0.11          |
| (1,629) | 1:106:A:ILE:HD12 | 1:57:A:MET:HE1  | 12       | 0.11          |
| (1,629) | 1:106:A:ILE:HD12 | 1:57:A:MET:HE2  | 12       | 0.11          |
| (1,629) | 1:106:A:ILE:HD12 | 1:57:A:MET:HE3  | 12       | 0.11          |
| (1,629) | 1:106:A:ILE:HD13 | 1:57:A:MET:HE1  | 12       | 0.11          |
| (1,629) | 1:106:A:ILE:HD13 | 1:57:A:MET:HE2  | 12       | 0.11          |
| (1,629) | 1:106:A:ILE:HD13 | 1:57:A:MET:HE3  | 12       | 0.11          |
| (1,426) | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG21 | 4        | 0.11          |
| (1,426) | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG22 | 4        | 0.11          |
| (1,426) | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG23 | 4        | 0.11          |
| (1,426) | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG21 | 4        | 0.11          |
| (1,426) | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG22 | 4        | 0.11          |
| (1,426) | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG23 | 4        | 0.11          |
| (1,426) | 1:79:A:VAL:HG23  | 1:92:A:ILE:HG21 | 4        | 0.11          |
| (1,426) | 1:79:A:VAL:HG23  | 1:92:A:ILE:HG22 | 4        | 0.11          |
| (1,426) | 1:79:A:VAL:HG23  | 1:92:A:ILE:HG23 | 4        | 0.11          |
| (1,426) | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG21 | 8        | 0.11          |
| (1,426) | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG22 | 8        | 0.11          |
| (1,426) | 1:79:A:VAL:HG21  | 1:92:A:ILE:HG23 | 8        | 0.11          |
| (1,426) | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG21 | 8        | 0.11          |
| (1,426) | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG22 | 8        | 0.11          |
| (1,426) | 1:79:A:VAL:HG22  | 1:92:A:ILE:HG23 | 8        | 0.11          |
| (1,426) | 1:79:A:VAL:HG23  | 1:92:A:ILE:HG21 | 8        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,426)  | 1:79:A:VAL:HG23 | 1:92:A:ILE:HG22 | 8        | 0.11          |
| (1,426)  | 1:79:A:VAL:HG23 | 1:92:A:ILE:HG23 | 8        | 0.11          |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG2  | 18       | 0.11          |
| (1,334)  | 1:66:A:LEU:HD11 | 1:94:A:MET:HG3  | 18       | 0.11          |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG2  | 18       | 0.11          |
| (1,334)  | 1:66:A:LEU:HD12 | 1:94:A:MET:HG3  | 18       | 0.11          |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG2  | 18       | 0.11          |
| (1,334)  | 1:66:A:LEU:HD13 | 1:94:A:MET:HG3  | 18       | 0.11          |
| (1,263)  | 1:58:A:THR:HB   | 1:60:A:TYR:HA   | 16       | 0.11          |
| (1,199)  | 1:55:A:PRO:HA   | 1:118:A:TRP:HZ2 | 2        | 0.11          |
| (1,197)  | 1:54:A:THR:HG21 | 1:56:A:TYR:HD1  | 20       | 0.11          |
| (1,197)  | 1:54:A:THR:HG21 | 1:56:A:TYR:HD2  | 20       | 0.11          |
| (1,197)  | 1:54:A:THR:HG22 | 1:56:A:TYR:HD1  | 20       | 0.11          |
| (1,197)  | 1:54:A:THR:HG22 | 1:56:A:TYR:HD2  | 20       | 0.11          |
| (1,197)  | 1:54:A:THR:HG23 | 1:56:A:TYR:HD1  | 20       | 0.11          |
| (1,197)  | 1:54:A:THR:HG23 | 1:56:A:TYR:HD2  | 20       | 0.11          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2  | 5        | 0.11          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3  | 5        | 0.11          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2  | 5        | 0.11          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3  | 5        | 0.11          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2  | 5        | 0.11          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3  | 5        | 0.11          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2  | 19       | 0.11          |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3  | 19       | 0.11          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2  | 19       | 0.11          |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3  | 19       | 0.11          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2  | 19       | 0.11          |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3  | 19       | 0.11          |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE1 | 20       | 0.11          |
| (1,80)   | 1:37:A:GLU:HB2  | 1:109:A:TYR:HE2 | 20       | 0.11          |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE1 | 20       | 0.11          |
| (1,80)   | 1:37:A:GLU:HB3  | 1:109:A:TYR:HE2 | 20       | 0.11          |
| (2,39)   | 1:91:A:LEU:O    | 1:95:A:LYS:H    | 19       | 0.1           |
| (1,1534) | 1:57:A:MET:H    | 1:57:A:MET:HB2  | 2        | 0.1           |
| (1,1534) | 1:57:A:MET:H    | 1:57:A:MET:HB2  | 6        | 0.1           |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB  | 19       | 0.1           |
| (1,1498) | 1:126:A:THR:H   | 1:125:A:ILE:HB  | 20       | 0.1           |
| (1,1492) | 1:124:A:ILE:H   | 1:123:A:LEU:HG  | 18       | 0.1           |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA  | 4        | 0.1           |
| (1,1313) | 1:102:A:ILE:H   | 1:101:A:LYS:HA  | 11       | 0.1           |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA   | 1        | 0.1           |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA   | 10       | 0.1           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA    | 12       | 0.1           |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA    | 16       | 0.1           |
| (1,1125) | 1:71:A:LEU:H    | 1:69:A:ARG:HA    | 20       | 0.1           |
| (1,1066) | 1:63:A:ALA:H    | 1:61:A:GLU:HB2   | 13       | 0.1           |
| (1,939)  | 1:39:A:LEU:H    | 1:104:A:ILE:HA   | 1        | 0.1           |
| (1,939)  | 1:39:A:LEU:H    | 1:104:A:ILE:HA   | 3        | 0.1           |
| (1,930)  | 1:38:A:ILE:H    | 1:36:A:VAL:HA    | 12       | 0.1           |
| (1,608)  | 1:105:A:ILE:HB  | 1:117:A:ASP:HA   | 8        | 0.1           |
| (1,478)  | 1:87:A:THR:HB   | 1:83:A:LEU:HG    | 2        | 0.1           |
| (1,478)  | 1:87:A:THR:HB   | 1:83:A:LEU:HG    | 3        | 0.1           |
| (1,478)  | 1:87:A:THR:HB   | 1:83:A:LEU:HG    | 14       | 0.1           |
| (1,478)  | 1:87:A:THR:HB   | 1:83:A:LEU:HG    | 15       | 0.1           |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD2  | 4        | 0.1           |
| (1,442)  | 1:81:A:VAL:HG11 | 1:101:A:LYS:HD3  | 4        | 0.1           |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD2  | 4        | 0.1           |
| (1,442)  | 1:81:A:VAL:HG12 | 1:101:A:LYS:HD3  | 4        | 0.1           |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD2  | 4        | 0.1           |
| (1,442)  | 1:81:A:VAL:HG13 | 1:101:A:LYS:HD3  | 4        | 0.1           |
| (1,419)  | 1:79:A:VAL:HA   | 1:92:A:ILE:HB    | 14       | 0.1           |
| (1,199)  | 1:55:A:PRO:HA   | 1:118:A:TRP:HZ2  | 20       | 0.1           |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG12 | 6        | 0.1           |
| (1,121)  | 1:41:A:SER:HB3  | 1:105:A:ILE:HG13 | 6        | 0.1           |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB2   | 10       | 0.1           |
| (1,91)   | 1:38:A:ILE:HD11 | 1:64:A:ARG:HB3   | 10       | 0.1           |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB2   | 10       | 0.1           |
| (1,91)   | 1:38:A:ILE:HD12 | 1:64:A:ARG:HB3   | 10       | 0.1           |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB2   | 10       | 0.1           |
| (1,91)   | 1:38:A:ILE:HD13 | 1:64:A:ARG:HB3   | 10       | 0.1           |



## 10 Dihedral-angle violation analysis ⓘ

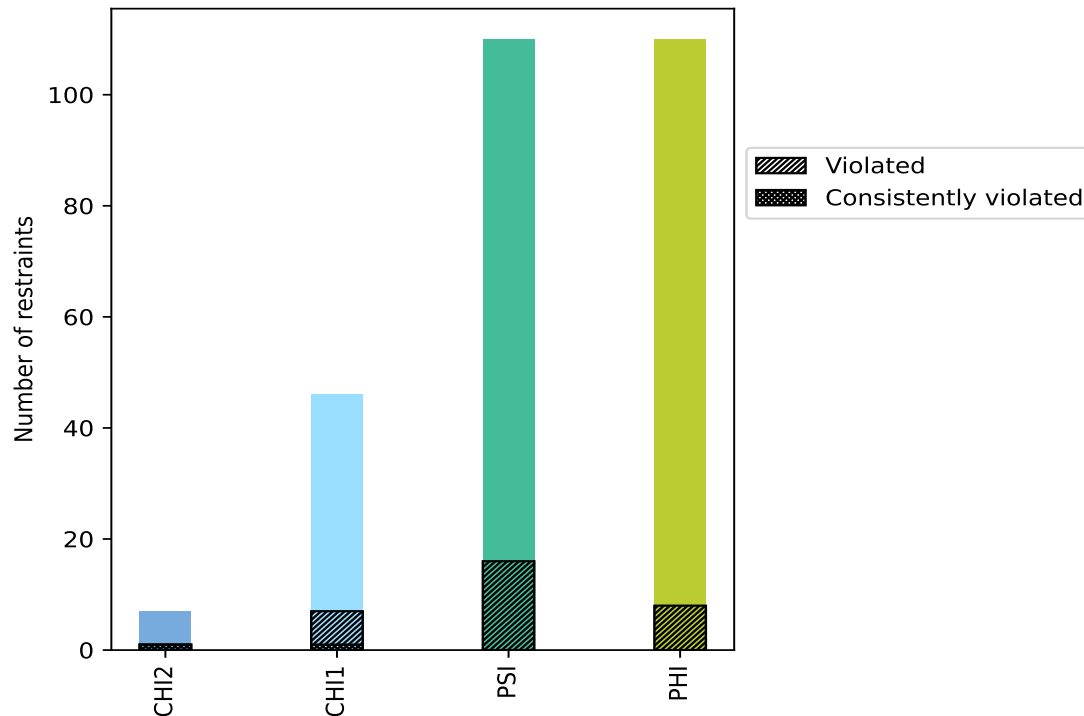
### 10.1 Summary of dihedral-angle violations ⓘ

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| CHI2       | 7     | 2.6            | 1                     | 14.3           | 0.4            | 1                                  | 14.3           | 0.4            |
| CHI1       | 46    | 16.8           | 7                     | 15.2           | 2.6            | 1                                  | 2.2            | 0.4            |
| PSI        | 110   | 40.3           | 16                    | 14.5           | 5.9            | 0                                  | 0.0            | 0.0            |
| PHI        | 110   | 40.3           | 8                     | 7.3            | 2.9            | 0                                  | 0.0            | 0.0            |
| Total      | 273   | 100.0          | 32                    | 11.7           | 11.7           | 2                                  | 0.7            | 0.7            |

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

#### 10.1.1 Bar chart : Distribution of dihedral-angles and violations ⓘ



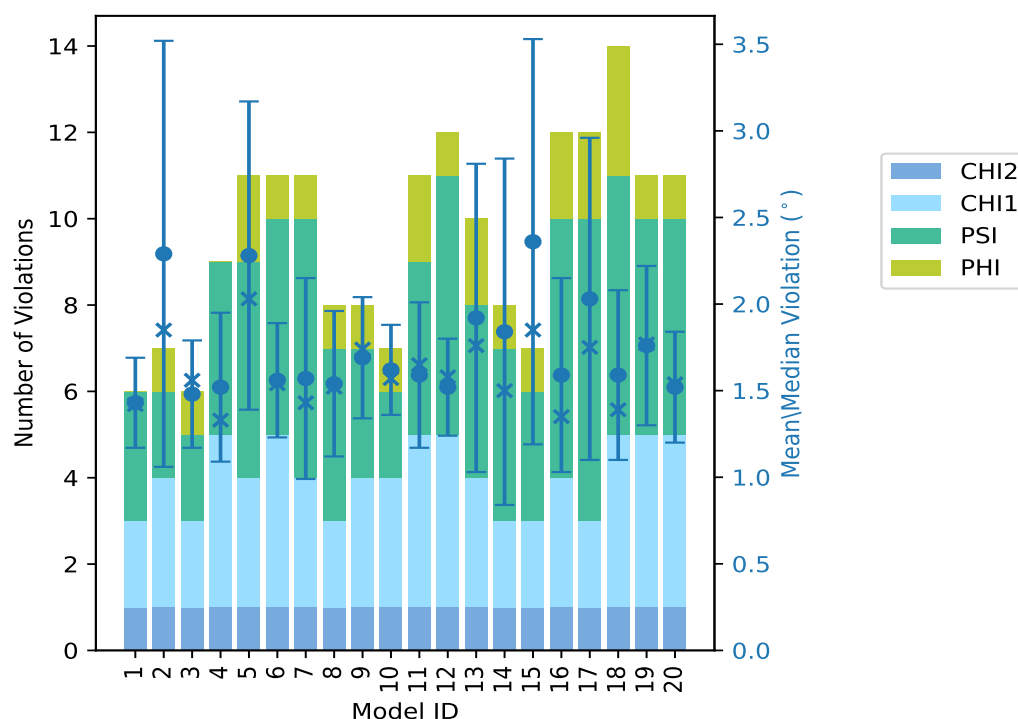
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |      |     |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|------|-----|-----|-------|----------|---------|--------|------------|
|          | CHI2                 | CHI1 | PSI | PHI | Total |          |         |        |            |
| 1        | 1                    | 2    | 3   | 0   | 6     | 1.43     | 1.72    | 0.26   | 1.42       |
| 2        | 1                    | 3    | 2   | 1   | 7     | 2.29     | 4.74    | 1.23   | 1.85       |
| 3        | 1                    | 2    | 2   | 1   | 6     | 1.48     | 1.92    | 0.31   | 1.56       |
| 4        | 1                    | 4    | 4   | 0   | 9     | 1.52     | 2.57    | 0.43   | 1.33       |
| 5        | 1                    | 3    | 5   | 2   | 11    | 2.28     | 3.67    | 0.89   | 2.03       |
| 6        | 1                    | 4    | 5   | 1   | 11    | 1.56     | 2.32    | 0.33   | 1.54       |
| 7        | 1                    | 3    | 6   | 1   | 11    | 1.57     | 3.17    | 0.58   | 1.43       |
| 8        | 1                    | 2    | 4   | 1   | 8     | 1.54     | 2.37    | 0.42   | 1.52       |
| 9        | 1                    | 3    | 3   | 1   | 8     | 1.69     | 2.16    | 0.35   | 1.74       |
| 10       | 1                    | 3    | 2   | 1   | 7     | 1.62     | 2.04    | 0.26   | 1.57       |
| 11       | 1                    | 4    | 4   | 2   | 11    | 1.59     | 2.37    | 0.42   | 1.65       |
| 12       | 1                    | 4    | 6   | 1   | 12    | 1.52     | 2.01    | 0.28   | 1.58       |
| 13       | 1                    | 3    | 4   | 2   | 10    | 1.92     | 4.19    | 0.89   | 1.76       |
| 14       | 1                    | 2    | 4   | 1   | 8     | 1.84     | 4.3     | 1.0    | 1.5        |
| 15       | 1                    | 2    | 3   | 1   | 7     | 2.36     | 4.63    | 1.17   | 1.85       |
| 16       | 1                    | 3    | 6   | 2   | 12    | 1.59     | 2.58    | 0.56   | 1.35       |
| 17       | 1                    | 2    | 7   | 2   | 12    | 2.03     | 4.31    | 0.93   | 1.75       |
| 18       | 1                    | 4    | 6   | 3   | 14    | 1.59     | 2.68    | 0.49   | 1.39       |
| 19       | 1                    | 4    | 5   | 1   | 11    | 1.76     | 2.85    | 0.46   | 1.77       |
| 20       | 1                    | 4    | 5   | 1   | 11    | 1.52     | 2.02    | 0.32   | 1.54       |

### 10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

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

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

| Number of violated restraints |      |     |     |       | Fraction of the ensemble |      |
|-------------------------------|------|-----|-----|-------|--------------------------|------|
| CHI2                          | CHI1 | PSI | PHI | Total | Count <sup>1</sup>       | %    |
| 0                             | 0    | 6   | 1   | 7     | 1                        | 5.0  |
| 0                             | 2    | 2   | 4   | 8     | 2                        | 10.0 |
| 0                             | 1    | 0   | 1   | 2     | 3                        | 15.0 |
| 0                             | 0    | 0   | 0   | 0     | 4                        | 20.0 |
| 0                             | 0    | 0   | 0   | 0     | 5                        | 25.0 |
| 0                             | 0    | 2   | 1   | 3     | 6                        | 30.0 |
| 0                             | 0    | 2   | 1   | 3     | 7                        | 35.0 |
| 0                             | 1    | 1   | 0   | 2     | 8                        | 40.0 |
| 0                             | 0    | 0   | 0   | 0     | 9                        | 45.0 |
| 0                             | 0    | 0   | 0   | 0     | 10                       | 50.0 |
| 0                             | 0    | 1   | 0   | 1     | 11                       | 55.0 |

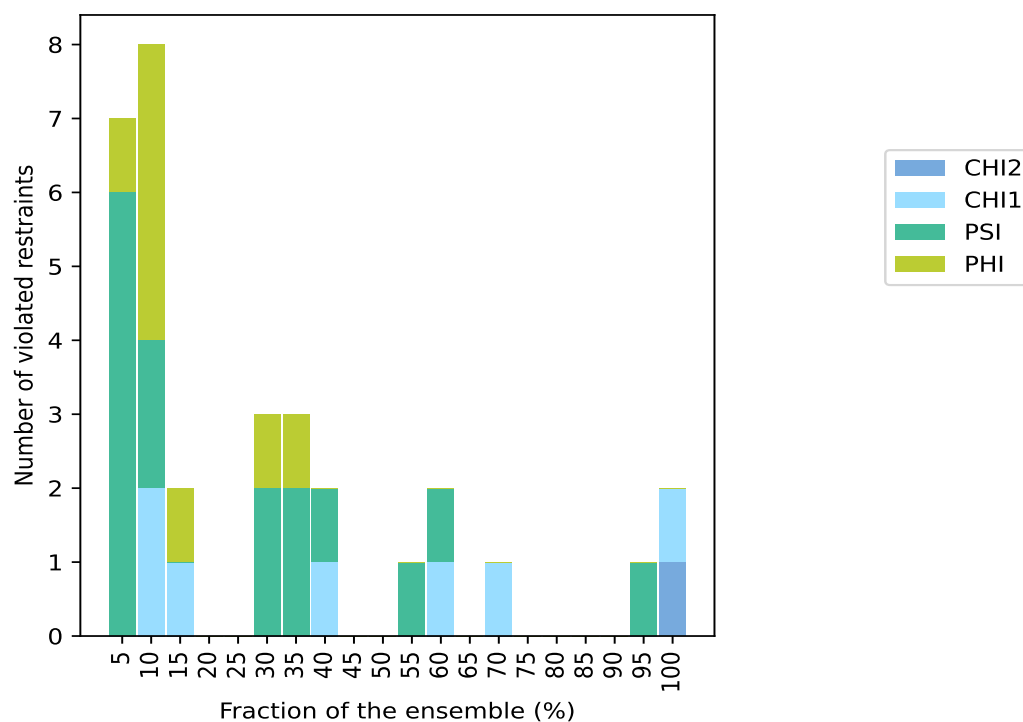
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| Number of violated restraints |      |     |     |       | Fraction of the ensemble |       |
|-------------------------------|------|-----|-----|-------|--------------------------|-------|
| CHI2                          | CHI1 | PSI | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 1    | 1   | 0   | 2     | 12                       | 60.0  |
| 0                             | 0    | 0   | 0   | 0     | 13                       | 65.0  |
| 0                             | 1    | 0   | 0   | 1     | 14                       | 70.0  |
| 0                             | 0    | 0   | 0   | 0     | 15                       | 75.0  |
| 0                             | 0    | 0   | 0   | 0     | 16                       | 80.0  |
| 0                             | 0    | 0   | 0   | 0     | 17                       | 85.0  |
| 0                             | 0    | 0   | 0   | 0     | 18                       | 90.0  |
| 0                             | 0    | 1   | 0   | 1     | 19                       | 95.0  |
| 1                             | 1    | 0   | 0   | 2     | 20                       | 100.0 |

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

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

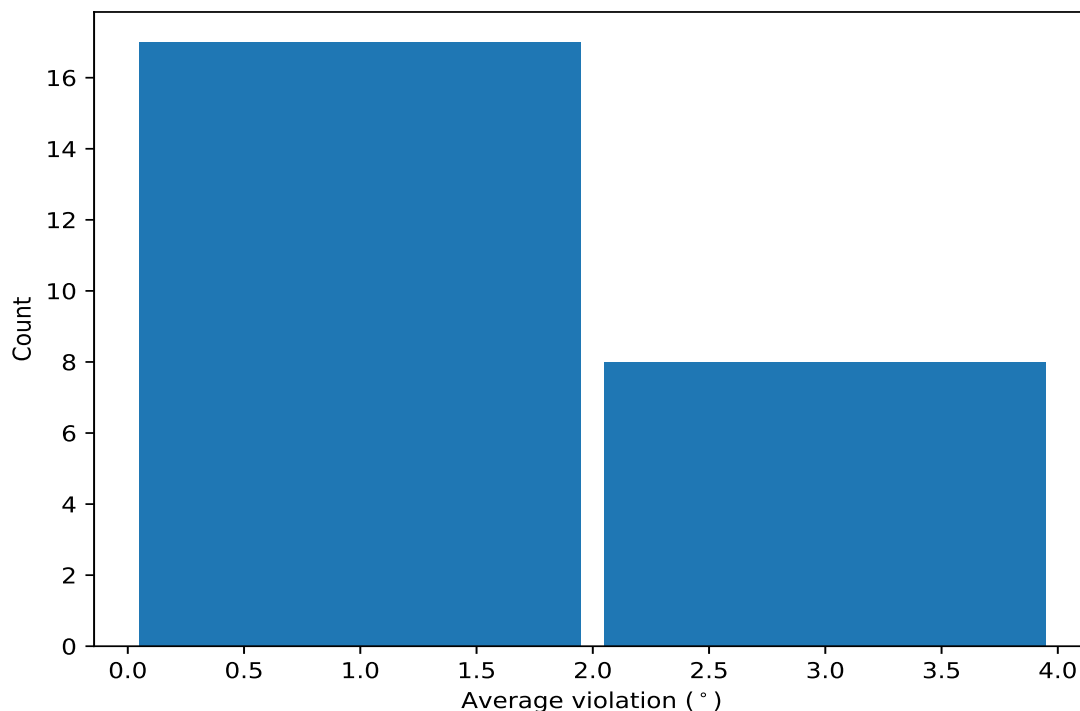


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4         | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|----------------|---------------------|------|-----------------|--------|
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 20                  | 1.88 | 0.24            | 1.84   |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 20                  | 1.73 | 0.12            | 1.74   |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 19                  | 1.71 | 0.33            | 1.71   |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB  | 1:83:A:LEU:CG  | 14                  | 1.3  | 0.21            | 1.29   |
| (1,252) | 1:53:A:THR:N  | 1:53:A:THR:CA  | 1:53:A:THR:CB  | 1:53:A:THR:OG1 | 12                  | 1.52 | 0.33            | 1.57   |
| (1,178) | 1:103:A:PRO:N | 1:103:A:PRO:CA | 1:103:A:PRO:C  | 1:104:A:ILE:N  | 12                  | 1.23 | 0.14            | 1.23   |
| (1,56)  | 1:33:A:GLN:N  | 1:33:A:GLN:CA  | 1:33:A:GLN:C   | 1:34:A:GLU:N   | 11                  | 2.17 | 0.86            | 2.01   |
| (1,2)   | 1:2:A:SER:N   | 1:2:A:SER:CA   | 1:2:A:SER:C    | 1:3:A:ASP:N    | 8                   | 2.88 | 1.36            | 2.48   |
| (1,223) | 1:39:A:LEU:N  | 1:39:A:LEU:CA  | 1:39:A:LEU:CB  | 1:39:A:LEU:CG  | 8                   | 1.26 | 0.17            | 1.27   |
| (1,75)  | 1:45:A:PRO:N  | 1:45:A:PRO:CA  | 1:45:A:PRO:C   | 1:46:A:GLN:N   | 7                   | 2.33 | 1.04            | 2.02   |
| (1,76)  | 1:45:A:PRO:C  | 1:46:A:GLN:N   | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 7                   | 2.05 | 1.0             | 1.56   |
| (1,24)  | 1:13:A:PHE:N  | 1:13:A:PHE:CA  | 1:13:A:PHE:C   | 1:14:A:ASP:N   | 7                   | 1.31 | 0.19            | 1.29   |
| (1,77)  | 1:46:A:GLN:N  | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 1:47:A:ALA:N   | 6                   | 2.39 | 0.81            | 2.32   |
| (1,3)   | 1:2:A:SER:C   | 1:3:A:ASP:N    | 1:3:A:ASP:CA   | 1:3:A:ASP:C    | 6                   | 2.37 | 0.75            | 2.58   |
| (1,81)  | 1:48:A:ASN:N  | 1:48:A:ASN:CA  | 1:48:A:ASN:C   | 1:49:A:GLN:N   | 6                   | 1.56 | 0.54            | 1.4    |
| (1,78)  | 1:46:A:GLN:C  | 1:47:A:ALA:N   | 1:47:A:ALA:CA  | 1:47:A:ALA:C   | 3                   | 2.23 | 0.25            | 2.39   |
| (1,253) | 1:58:A:THR:N  | 1:58:A:THR:CA  | 1:58:A:THR:CB  | 1:58:A:THR:OG1 | 3                   | 2.08 | 0.61            | 2.03   |
| (1,86)  | 1:50:A:LYS:C  | 1:51:A:ARG:N   | 1:51:A:ARG:CA  | 1:51:A:ARG:C   | 2                   | 1.52 | 0.52            | 1.52   |
| (1,45)  | 1:23:A:ASP:C  | 1:24:A:ASP:N   | 1:24:A:ASP:CA  | 1:24:A:ASP:C   | 2                   | 1.48 | 0.05            | 1.48   |
| (1,256) | 1:36:A:VAL:N  | 1:36:A:VAL:CA  | 1:36:A:VAL:CB  | 1:36:A:VAL:CG1 | 2                   | 1.38 | 0.3             | 1.38   |

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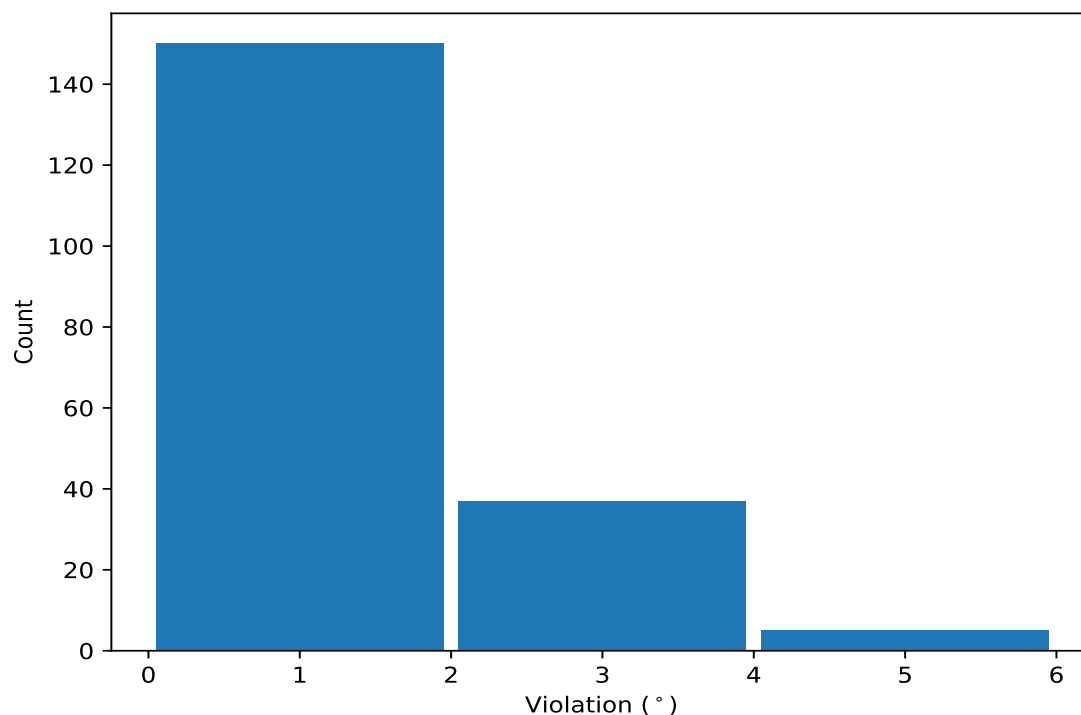
| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|---------------|---------------------|------|-----------------|--------|
| (1,96)  | 1:60:A:TYR:N | 1:60:A:TYR:CA | 1:60:A:TYR:C  | 1:61:A:GLU:N  | 2                   | 1.22 | 0.12            | 1.22   |
| (1,224) | 1:56:A:TYR:N | 1:56:A:TYR:CA | 1:56:A:TYR:CB | 1:56:A:TYR:CG | 2                   | 1.14 | 0.03            | 1.14   |
| (1,73)  | 1:44:A:ARG:N | 1:44:A:ARG:CA | 1:44:A:ARG:C  | 1:45:A:PRO:N  | 2                   | 1.12 | 0.03            | 1.12   |
| (1,145) | 1:84:A:GLU:C | 1:85:A:GLY:N  | 1:85:A:GLY:CA | 1:85:A:GLY:C  | 2                   | 1.06 | 0.03            | 1.06   |
| (1,5)   | 1:3:A:ASP:C  | 1:4:A:ASN:N   | 1:4:A:ASN:CA  | 1:4:A:ASN:C   | 2                   | 1.02 | 0.01            | 1.02   |

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

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

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

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



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

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

| Key   | Atom-1      | Atom-2       | Atom-3      | Atom-4      | Model ID | Violation (°) |
|-------|-------------|--------------|-------------|-------------|----------|---------------|
| (1,2) | 1:2:A:SER:N | 1:2:A:SER:CA | 1:2:A:SER:C | 1:3:A:ASP:N | 2        | 4.74          |
| (1,2) | 1:2:A:SER:N | 1:2:A:SER:CA | 1:2:A:SER:C | 1:3:A:ASP:N | 15       | 4.63          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4         | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|----------------|----------|---------------|
| (1,75)  | 1:45:A:PRO:N  | 1:45:A:PRO:CA  | 1:45:A:PRO:C   | 1:46:A:GLN:N   | 17       | 4.31          |
| (1,56)  | 1:33:A:GLN:N  | 1:33:A:GLN:CA  | 1:33:A:GLN:C   | 1:34:A:GLU:N   | 14       | 4.3           |
| (1,2)   | 1:2:A:SER:N   | 1:2:A:SER:CA   | 1:2:A:SER:C    | 1:3:A:ASP:N    | 13       | 4.19          |
| (1,76)  | 1:45:A:PRO:C  | 1:46:A:GLN:N   | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 5        | 3.67          |
| (1,76)  | 1:45:A:PRO:C  | 1:46:A:GLN:N   | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 17       | 3.54          |
| (1,77)  | 1:46:A:GLN:N  | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 1:47:A:ALA:N   | 5        | 3.52          |
| (1,75)  | 1:45:A:PRO:N  | 1:45:A:PRO:CA  | 1:45:A:PRO:C   | 1:46:A:GLN:N   | 5        | 3.42          |
| (1,3)   | 1:2:A:SER:C   | 1:3:A:ASP:N    | 1:3:A:ASP:CA   | 1:3:A:ASP:C    | 2        | 3.32          |
| (1,77)  | 1:46:A:GLN:N  | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 1:47:A:ALA:N   | 7        | 3.17          |
| (1,56)  | 1:33:A:GLN:N  | 1:33:A:GLN:CA  | 1:33:A:GLN:C   | 1:34:A:GLU:N   | 15       | 3.12          |
| (1,3)   | 1:2:A:SER:C   | 1:3:A:ASP:N    | 1:3:A:ASP:CA   | 1:3:A:ASP:C    | 15       | 2.93          |
| (1,253) | 1:58:A:THR:N  | 1:58:A:THR:CA  | 1:58:A:THR:CB  | 1:58:A:THR:OG1 | 19       | 2.85          |
| (1,77)  | 1:46:A:GLN:N  | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 1:47:A:ALA:N   | 18       | 2.68          |
| (1,81)  | 1:48:A:ASN:N  | 1:48:A:ASN:CA  | 1:48:A:ASN:C   | 1:49:A:GLN:N   | 5        | 2.65          |
| (1,3)   | 1:2:A:SER:C   | 1:3:A:ASP:N    | 1:3:A:ASP:CA   | 1:3:A:ASP:C    | 13       | 2.64          |
| (1,2)   | 1:2:A:SER:N   | 1:2:A:SER:CA   | 1:2:A:SER:C    | 1:3:A:ASP:N    | 16       | 2.58          |
| (1,56)  | 1:33:A:GLN:N  | 1:33:A:GLN:CA  | 1:33:A:GLN:C   | 1:34:A:GLU:N   | 4        | 2.57          |
| (1,3)   | 1:2:A:SER:C   | 1:3:A:ASP:N    | 1:3:A:ASP:CA   | 1:3:A:ASP:C    | 16       | 2.51          |
| (1,78)  | 1:46:A:GLN:C  | 1:47:A:ALA:N   | 1:47:A:ALA:CA  | 1:47:A:ALA:C   | 17       | 2.41          |
| (1,78)  | 1:46:A:GLN:C  | 1:47:A:ALA:N   | 1:47:A:ALA:CA  | 1:47:A:ALA:C   | 5        | 2.39          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 8        | 2.37          |
| (1,2)   | 1:2:A:SER:N   | 1:2:A:SER:CA   | 1:2:A:SER:C    | 1:3:A:ASP:N    | 11       | 2.37          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 18       | 2.34          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 6        | 2.32          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 2        | 2.25          |
| (1,2)   | 1:2:A:SER:N   | 1:2:A:SER:CA   | 1:2:A:SER:C    | 1:3:A:ASP:N    | 9        | 2.16          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 14       | 2.13          |
| (1,56)  | 1:33:A:GLN:N  | 1:33:A:GLN:CA  | 1:33:A:GLN:C   | 1:34:A:GLU:N   | 17       | 2.1           |
| (1,75)  | 1:45:A:PRO:N  | 1:45:A:PRO:CA  | 1:45:A:PRO:C   | 1:46:A:GLN:N   | 19       | 2.09          |
| (1,56)  | 1:33:A:GLN:N  | 1:33:A:GLN:CA  | 1:33:A:GLN:C   | 1:34:A:GLU:N   | 9        | 2.09          |
| (1,252) | 1:53:A:THR:N  | 1:53:A:THR:CA  | 1:53:A:THR:CB  | 1:53:A:THR:OG1 | 13       | 2.06          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 7        | 2.05          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 16       | 2.04          |
| (1,86)  | 1:50:A:LYS:C  | 1:51:A:ARG:N   | 1:51:A:ARG:CA  | 1:51:A:ARG:C   | 10       | 2.04          |
| (1,253) | 1:58:A:THR:N  | 1:58:A:THR:CA  | 1:58:A:THR:CB  | 1:58:A:THR:OG1 | 5        | 2.03          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 18       | 2.03          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 11       | 2.02          |
| (1,75)  | 1:45:A:PRO:N  | 1:45:A:PRO:CA  | 1:45:A:PRO:C   | 1:46:A:GLN:N   | 20       | 2.02          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 13       | 2.01          |
| (1,56)  | 1:33:A:GLN:N  | 1:33:A:GLN:CA  | 1:33:A:GLN:C   | 1:34:A:GLU:N   | 12       | 2.01          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 19       | 1.98          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 16       | 1.96          |
| (1,77)  | 1:46:A:GLN:N  | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 1:47:A:ALA:N   | 20       | 1.96          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 17       | 1.93          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 3        | 1.92          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 14       | 1.92          |
| (1,252) | 1:53:A:THR:N  | 1:53:A:THR:CA  | 1:53:A:THR:CB  | 1:53:A:THR:OG1 | 19       | 1.91          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 10       | 1.89          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 9        | 1.88          |
| (1,78)  | 1:46:A:GLN:C  | 1:47:A:ALA:N   | 1:47:A:ALA:CA  | 1:47:A:ALA:C   | 18       | 1.88          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 4        | 1.87          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4         | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|----------------|----------|---------------|
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 11       | 1.86          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 2        | 1.85          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 16       | 1.85          |
| (1,252) | 1:53:A:THR:N  | 1:53:A:THR:CA  | 1:53:A:THR:CB  | 1:53:A:THR:OG1 | 11       | 1.85          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 6        | 1.85          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 15       | 1.85          |
| (1,56)  | 1:33:A:GLN:N  | 1:33:A:GLN:CA  | 1:33:A:GLN:C   | 1:34:A:GLU:N   | 19       | 1.85          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 8        | 1.84          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 6        | 1.83          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 5        | 1.83          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 18       | 1.8           |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB  | 1:83:A:LEU:CG  | 18       | 1.8           |
| (1,77)  | 1:46:A:GLN:N  | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 1:47:A:ALA:N   | 17       | 1.8           |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 13       | 1.79          |
| (1,3)   | 1:2:A:SER:C   | 1:3:A:ASP:N    | 1:3:A:ASP:CA   | 1:3:A:ASP:C    | 11       | 1.79          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 20       | 1.78          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 12       | 1.77          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 19       | 1.77          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 20       | 1.76          |
| (1,252) | 1:53:A:THR:N  | 1:53:A:THR:CA  | 1:53:A:THR:CB  | 1:53:A:THR:OG1 | 8        | 1.76          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 12       | 1.76          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 9        | 1.75          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 9        | 1.73          |
| (1,252) | 1:53:A:THR:N  | 1:53:A:THR:CA  | 1:53:A:THR:CB  | 1:53:A:THR:OG1 | 12       | 1.73          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 1        | 1.72          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 1        | 1.72          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 13       | 1.72          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 5        | 1.71          |
| (1,81)  | 1:48:A:ASN:N  | 1:48:A:ASN:CA  | 1:48:A:ASN:C   | 1:49:A:GLN:N   | 12       | 1.71          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 14       | 1.7           |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 17       | 1.7           |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 5        | 1.69          |
| (1,256) | 1:36:A:VAL:N  | 1:36:A:VAL:CA  | 1:36:A:VAL:CB  | 1:36:A:VAL:CG1 | 20       | 1.68          |
| (1,75)  | 1:45:A:PRO:N  | 1:45:A:PRO:CA  | 1:45:A:PRO:C   | 1:46:A:GLN:N   | 10       | 1.68          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 19       | 1.66          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 3        | 1.66          |
| (1,56)  | 1:33:A:GLN:N  | 1:33:A:GLN:CA  | 1:33:A:GLN:C   | 1:34:A:GLU:N   | 7        | 1.65          |
| (1,56)  | 1:33:A:GLN:N  | 1:33:A:GLN:CA  | 1:33:A:GLN:C   | 1:34:A:GLU:N   | 11       | 1.65          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 4        | 1.64          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 2        | 1.62          |
| (1,76)  | 1:45:A:PRO:C  | 1:46:A:GLN:N   | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 19       | 1.61          |
| (1,24)  | 1:13:A:PHE:N  | 1:13:A:PHE:CA  | 1:13:A:PHE:C   | 1:14:A:ASP:N   | 12       | 1.61          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 15       | 1.6           |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 3        | 1.6           |
| (1,223) | 1:39:A:LEU:N  | 1:39:A:LEU:CA  | 1:39:A:LEU:CB  | 1:39:A:LEU:CG  | 6        | 1.59          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 1        | 1.59          |
| (1,252) | 1:53:A:THR:N  | 1:53:A:THR:CA  | 1:53:A:THR:CB  | 1:53:A:THR:OG1 | 6        | 1.58          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 7        | 1.57          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 8        | 1.57          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 10       | 1.57          |
| (1,252) | 1:53:A:THR:N  | 1:53:A:THR:CA  | 1:53:A:THR:CB  | 1:53:A:THR:OG1 | 9        | 1.56          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4         | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|----------------|----------|---------------|
| (1,76)  | 1:45:A:PRO:C  | 1:46:A:GLN:N   | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 12       | 1.56          |
| (1,178) | 1:103:A:PRO:N | 1:103:A:PRO:CA | 1:103:A:PRO:C  | 1:104:A:ILE:N  | 6        | 1.54          |
| (1,76)  | 1:45:A:PRO:C  | 1:46:A:GLN:N   | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 20       | 1.54          |
| (1,75)  | 1:45:A:PRO:N  | 1:45:A:PRO:CA  | 1:45:A:PRO:C   | 1:46:A:GLN:N   | 6        | 1.54          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 10       | 1.52          |
| (1,45)  | 1:23:A:ASP:C  | 1:24:A:ASP:N   | 1:24:A:ASP:CA  | 1:24:A:ASP:C   | 3        | 1.52          |
| (1,270) | 1:90:A:LEU:CA | 1:90:A:LEU:CB  | 1:90:A:LEU:CG  | 1:90:A:LEU:CD1 | 17       | 1.49          |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB  | 1:83:A:LEU:CG  | 7        | 1.49          |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB  | 1:83:A:LEU:CG  | 11       | 1.48          |
| (1,24)  | 1:13:A:PHE:N  | 1:13:A:PHE:CA  | 1:13:A:PHE:C   | 1:14:A:ASP:N   | 8        | 1.48          |
| (1,81)  | 1:48:A:ASN:N  | 1:48:A:ASN:CA  | 1:48:A:ASN:C   | 1:49:A:GLN:N   | 17       | 1.47          |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB  | 1:83:A:LEU:CG  | 10       | 1.46          |
| (1,24)  | 1:13:A:PHE:N  | 1:13:A:PHE:CA  | 1:13:A:PHE:C   | 1:14:A:ASP:N   | 4        | 1.44          |
| (1,45)  | 1:23:A:ASP:C  | 1:24:A:ASP:N   | 1:24:A:ASP:CA  | 1:24:A:ASP:C   | 7        | 1.43          |
| (1,83)  | 1:49:A:GLN:N  | 1:49:A:GLN:CA  | 1:49:A:GLN:C   | 1:50:A:LYS:N   | 18       | 1.41          |
| (1,56)  | 1:33:A:GLN:N  | 1:33:A:GLN:CA  | 1:33:A:GLN:C   | 1:34:A:GLU:N   | 16       | 1.4           |
| (1,253) | 1:58:A:THR:N  | 1:58:A:THR:CA  | 1:58:A:THR:CB  | 1:58:A:THR:OG1 | 18       | 1.37          |
| (1,249) | 1:123:A:LEU:N | 1:123:A:LEU:CA | 1:123:A:LEU:CB | 1:123:A:LEU:CG | 11       | 1.37          |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB  | 1:83:A:LEU:CG  | 13       | 1.36          |
| (1,223) | 1:39:A:LEU:N  | 1:39:A:LEU:CA  | 1:39:A:LEU:CB  | 1:39:A:LEU:CG  | 18       | 1.36          |
| (1,178) | 1:103:A:PRO:N | 1:103:A:PRO:CA | 1:103:A:PRO:C  | 1:104:A:ILE:N  | 18       | 1.36          |
| (1,96)  | 1:60:A:TYR:N  | 1:60:A:TYR:CA  | 1:60:A:TYR:C   | 1:61:A:GLU:N   | 19       | 1.34          |
| (1,76)  | 1:45:A:PRO:C  | 1:46:A:GLN:N   | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 6        | 1.34          |
| (1,223) | 1:39:A:LEU:N  | 1:39:A:LEU:CA  | 1:39:A:LEU:CB  | 1:39:A:LEU:CG  | 4        | 1.33          |
| (1,178) | 1:103:A:PRO:N | 1:103:A:PRO:CA | 1:103:A:PRO:C  | 1:104:A:ILE:N  | 20       | 1.33          |
| (1,81)  | 1:48:A:ASN:N  | 1:48:A:ASN:CA  | 1:48:A:ASN:C   | 1:49:A:GLN:N   | 7        | 1.33          |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB  | 1:83:A:LEU:CG  | 9        | 1.31          |
| (1,223) | 1:39:A:LEU:N  | 1:39:A:LEU:CA  | 1:39:A:LEU:CB  | 1:39:A:LEU:CG  | 12       | 1.31          |
| (1,178) | 1:103:A:PRO:N | 1:103:A:PRO:CA | 1:103:A:PRO:C  | 1:104:A:ILE:N  | 16       | 1.3           |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB  | 1:83:A:LEU:CG  | 16       | 1.29          |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB  | 1:83:A:LEU:CG  | 20       | 1.29          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 4        | 1.29          |
| (1,24)  | 1:13:A:PHE:N  | 1:13:A:PHE:CA  | 1:13:A:PHE:C   | 1:14:A:ASP:N   | 14       | 1.29          |
| (1,178) | 1:103:A:PRO:N | 1:103:A:PRO:CA | 1:103:A:PRO:C  | 1:104:A:ILE:N  | 19       | 1.26          |
| (1,204) | 1:118:A:TRP:N | 1:118:A:TRP:CA | 1:118:A:TRP:C  | 1:119:A:GLY:N  | 1        | 1.25          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C  | 1:108:A:ARG:N  | 12       | 1.25          |
| (1,2)   | 1:2:A:SER:N   | 1:2:A:SER:CA   | 1:2:A:SER:C    | 1:3:A:ASP:N    | 6        | 1.25          |
| (1,252) | 1:53:A:THR:N  | 1:53:A:THR:CA  | 1:53:A:THR:CB  | 1:53:A:THR:OG1 | 14       | 1.24          |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB  | 1:83:A:LEU:CG  | 17       | 1.24          |
| (1,178) | 1:103:A:PRO:N | 1:103:A:PRO:CA | 1:103:A:PRO:C  | 1:104:A:ILE:N  | 7        | 1.24          |
| (1,223) | 1:39:A:LEU:N  | 1:39:A:LEU:CA  | 1:39:A:LEU:CB  | 1:39:A:LEU:CG  | 15       | 1.23          |
| (1,34)  | 1:18:A:GLU:N  | 1:18:A:GLU:CA  | 1:18:A:GLU:C   | 1:19:A:ASP:N   | 1        | 1.23          |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB  | 1:83:A:LEU:CG  | 4        | 1.22          |
| (1,75)  | 1:45:A:PRO:N  | 1:45:A:PRO:CA  | 1:45:A:PRO:C   | 1:46:A:GLN:N   | 12       | 1.22          |
| (1,252) | 1:53:A:THR:N  | 1:53:A:THR:CA  | 1:53:A:THR:CB  | 1:53:A:THR:OG1 | 2        | 1.21          |
| (1,178) | 1:103:A:PRO:N | 1:103:A:PRO:CA | 1:103:A:PRO:C  | 1:104:A:ILE:N  | 13       | 1.21          |
| (1,223) | 1:39:A:LEU:N  | 1:39:A:LEU:CA  | 1:39:A:LEU:CB  | 1:39:A:LEU:CG  | 10       | 1.2           |
| (1,178) | 1:103:A:PRO:N | 1:103:A:PRO:CA | 1:103:A:PRO:C  | 1:104:A:ILE:N  | 17       | 1.2           |
| (1,24)  | 1:13:A:PHE:N  | 1:13:A:PHE:CA  | 1:13:A:PHE:C   | 1:14:A:ASP:N   | 17       | 1.2           |
| (1,77)  | 1:46:A:GLN:N  | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 1:47:A:ALA:N   | 6        | 1.19          |
| (1,6)   | 1:4:A:ASN:N   | 1:4:A:ASN:CA   | 1:4:A:ASN:C    | 1:5:A:GLU:N    | 8        | 1.19          |

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| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4         | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|----------------|----------|---------------|
| (1,252) | 1:53:A:THR:N  | 1:53:A:THR:CA  | 1:53:A:THR:CB | 1:53:A:THR:OG1 | 4        | 1.18          |
| (1,178) | 1:103:A:PRO:N | 1:103:A:PRO:CA | 1:103:A:PRO:C | 1:104:A:ILE:N  | 12       | 1.18          |
| (1,224) | 1:56:A:TYR:N  | 1:56:A:TYR:CA  | 1:56:A:TYR:CB | 1:56:A:TYR:CG  | 20       | 1.17          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C | 1:108:A:ARG:N  | 15       | 1.16          |
| (1,252) | 1:53:A:THR:N  | 1:53:A:THR:CA  | 1:53:A:THR:CB | 1:53:A:THR:OG1 | 7        | 1.15          |
| (1,202) | 1:117:A:ASP:N | 1:117:A:ASP:CA | 1:117:A:ASP:C | 1:118:A:TRP:N  | 8        | 1.15          |
| (1,81)  | 1:48:A:ASN:N  | 1:48:A:ASN:CA  | 1:48:A:ASN:C  | 1:49:A:GLN:N   | 20       | 1.15          |
| (1,73)  | 1:44:A:ARG:N  | 1:44:A:ARG:CA  | 1:44:A:ARG:C  | 1:45:A:PRO:N   | 13       | 1.15          |
| (1,2)   | 1:2:A:SER:N   | 1:2:A:SER:CA   | 1:2:A:SER:C   | 1:3:A:ASP:N    | 4        | 1.12          |
| (1,224) | 1:56:A:TYR:N  | 1:56:A:TYR:CA  | 1:56:A:TYR:CB | 1:56:A:TYR:CG  | 6        | 1.11          |
| (1,24)  | 1:13:A:PHE:N  | 1:13:A:PHE:CA  | 1:13:A:PHE:C  | 1:14:A:ASP:N   | 7        | 1.11          |
| (1,178) | 1:103:A:PRO:N | 1:103:A:PRO:CA | 1:103:A:PRO:C | 1:104:A:ILE:N  | 5        | 1.09          |
| (1,96)  | 1:60:A:TYR:N  | 1:60:A:TYR:CA  | 1:60:A:TYR:C  | 1:61:A:GLU:N   | 18       | 1.09          |
| (1,73)  | 1:44:A:ARG:N  | 1:44:A:ARG:CA  | 1:44:A:ARG:C  | 1:45:A:PRO:N   | 3        | 1.09          |
| (1,256) | 1:36:A:VAL:N  | 1:36:A:VAL:CA  | 1:36:A:VAL:CB | 1:36:A:VAL:CG1 | 5        | 1.08          |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB | 1:83:A:LEU:CG  | 12       | 1.08          |
| (1,145) | 1:84:A:GLU:C  | 1:85:A:GLY:N   | 1:85:A:GLY:CA | 1:85:A:GLY:C   | 14       | 1.08          |
| (1,56)  | 1:33:A:GLN:N  | 1:33:A:GLN:CA  | 1:33:A:GLN:C  | 1:34:A:GLU:N   | 20       | 1.08          |
| (1,47)  | 1:24:A:ASP:C  | 1:25:A:LEU:N   | 1:25:A:LEU:CA | 1:25:A:LEU:C   | 18       | 1.08          |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB | 1:83:A:LEU:CG  | 3        | 1.07          |
| (1,76)  | 1:45:A:PRO:C  | 1:46:A:GLN:N   | 1:46:A:GLN:CA | 1:46:A:GLN:C   | 18       | 1.06          |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB | 1:83:A:LEU:CG  | 1        | 1.05          |
| (1,186) | 1:107:A:ARG:N | 1:107:A:ARG:CA | 1:107:A:ARG:C | 1:108:A:ARG:N  | 7        | 1.05          |
| (1,178) | 1:103:A:PRO:N | 1:103:A:PRO:CA | 1:103:A:PRO:C | 1:104:A:ILE:N  | 14       | 1.05          |
| (1,252) | 1:53:A:THR:N  | 1:53:A:THR:CA  | 1:53:A:THR:CB | 1:53:A:THR:OG1 | 16       | 1.04          |
| (1,223) | 1:39:A:LEU:N  | 1:39:A:LEU:CA  | 1:39:A:LEU:CB | 1:39:A:LEU:CG  | 19       | 1.04          |
| (1,178) | 1:103:A:PRO:N | 1:103:A:PRO:CA | 1:103:A:PRO:C | 1:104:A:ILE:N  | 11       | 1.04          |
| (1,24)  | 1:13:A:PHE:N  | 1:13:A:PHE:CA  | 1:13:A:PHE:C  | 1:14:A:ASP:N   | 16       | 1.04          |
| (1,3)   | 1:2:A:SER:C   | 1:3:A:ASP:N    | 1:3:A:ASP:CA  | 1:3:A:ASP:C    | 9        | 1.04          |
| (1,145) | 1:84:A:GLU:C  | 1:85:A:GLY:N   | 1:85:A:GLY:CA | 1:85:A:GLY:C   | 11       | 1.03          |
| (1,81)  | 1:48:A:ASN:N  | 1:48:A:ASN:CA  | 1:48:A:ASN:C  | 1:49:A:GLN:N   | 18       | 1.03          |
| (1,5)   | 1:3:A:ASP:C   | 1:4:A:ASN:N    | 1:4:A:ASN:CA  | 1:4:A:ASN:C    | 13       | 1.03          |
| (1,223) | 1:39:A:LEU:N  | 1:39:A:LEU:CA  | 1:39:A:LEU:CB | 1:39:A:LEU:CG  | 11       | 1.02          |
| (1,5)   | 1:3:A:ASP:C   | 1:4:A:ASN:N    | 1:4:A:ASN:CA  | 1:4:A:ASN:C    | 16       | 1.02          |
| (1,232) | 1:83:A:LEU:N  | 1:83:A:LEU:CA  | 1:83:A:LEU:CB | 1:83:A:LEU:CG  | 2        | 1.01          |
| (1,86)  | 1:50:A:LYS:C  | 1:51:A:ARG:N   | 1:51:A:ARG:CA | 1:51:A:ARG:C   | 8        | 1.0           |
| (1,4)   | 1:3:A:ASP:N   | 1:3:A:ASP:CA   | 1:3:A:ASP:C   | 1:4:A:ASN:N    | 16       | 1.0           |