



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 07:40 AM UTC

PDB ID : 2LHI / pdb\_00002lhi  
BMRB ID : 17850  
Title : Solution structure of Ca<sup>2+</sup>/CNA1 peptide-bound yCaM  
Authors : Ogura, K.; Takahashi, K.; Kobashigawa, Y.; Yoshida, R.; Itoh, H.; Yazawa, M.; Inagaki, F.  
Deposited on : 2011-08-10

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

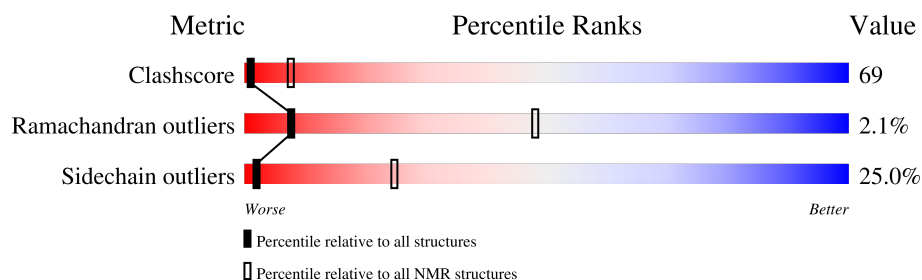
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

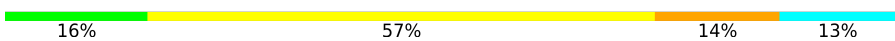
The overall completeness of chemical shifts assignment is 94%.

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     | 176    |  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 9 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:5-A:74, A:85-A:145,<br>A:455-A:476 (153) | 0.51              | 9            |

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

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

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

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2700 atoms, of which 1348 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 176      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2697  | 833 | 1348 | 231 | 280 | 5 |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 0       | GLY      | -      | expression tag | UNP P06787 |
| A     | 147     | GLY      | -      | linker         | UNP P06787 |
| A     | 148     | SER      | -      | linker         | UNP P06787 |
| A     | 149     | SER      | -      | linker         | UNP P06787 |
| A     | 150     | THR      | -      | linker         | UNP P06787 |
| A     | 151     | GLY      | -      | linker         | UNP P06787 |

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

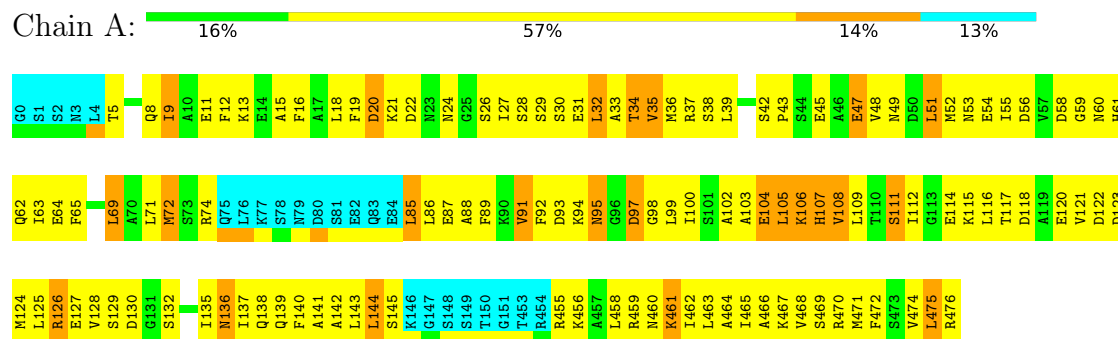
| Mol | Chain | Residues | Atoms |    |
|-----|-------|----------|-------|----|
| 2   | A     | 3        | Total | Ca |
|     |       |          | 3     | 3  |

## 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: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1

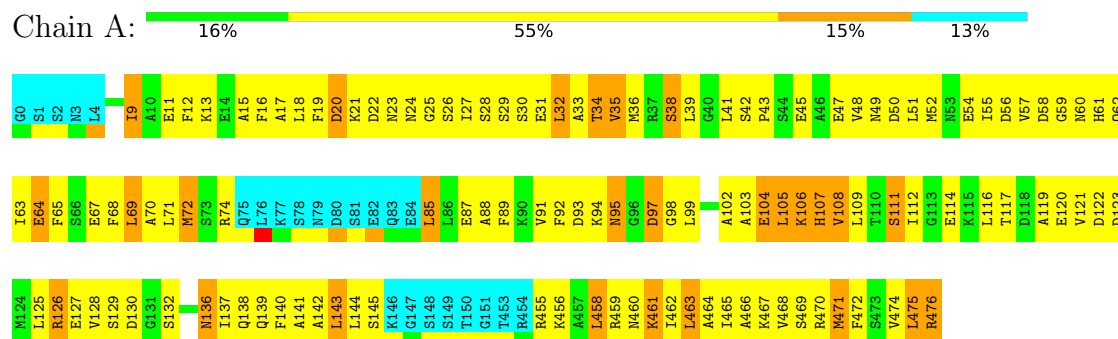


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



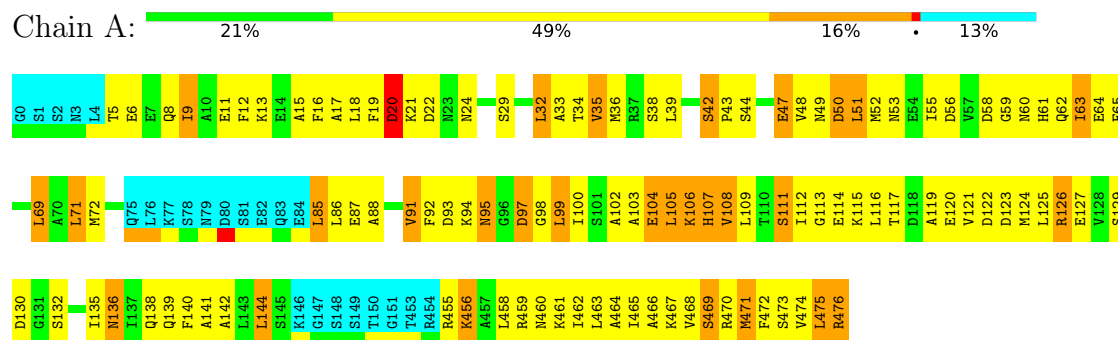
### 4.2.2 Score per residue for model 2

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



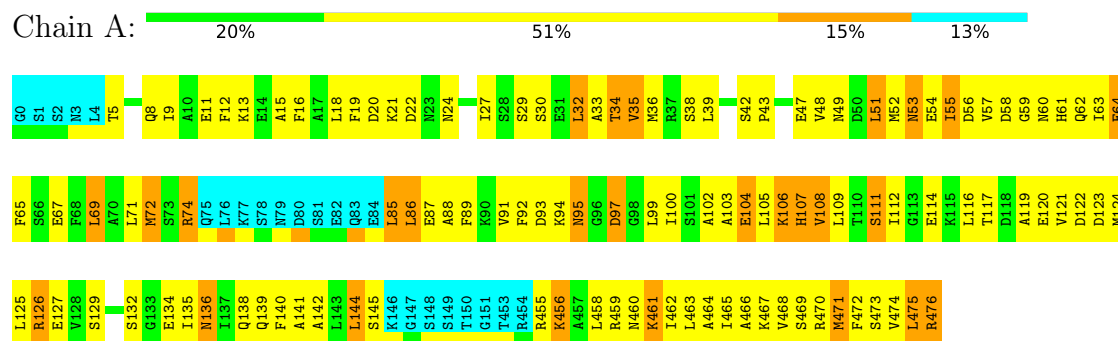
### 4.2.3 Score per residue for model 3

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



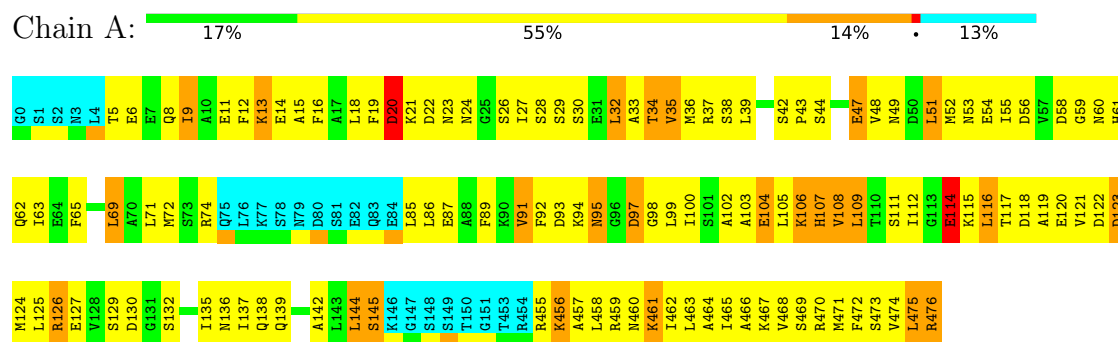
### 4.2.4 Score per residue for model 4

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



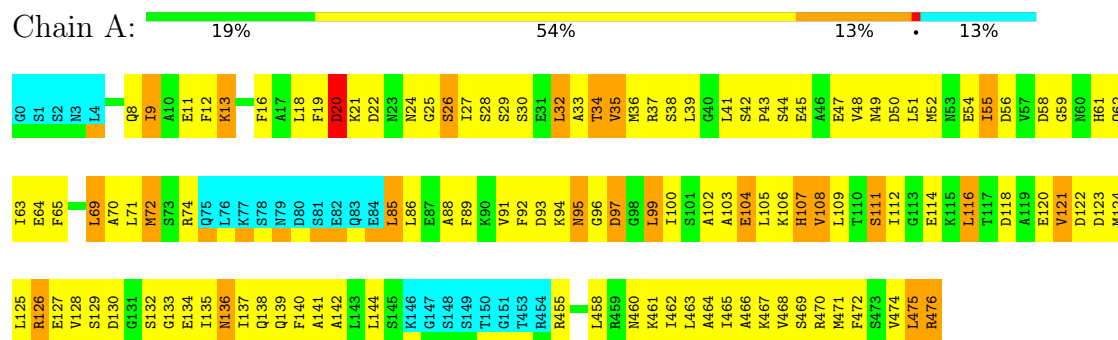
### 4.2.5 Score per residue for model 5

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



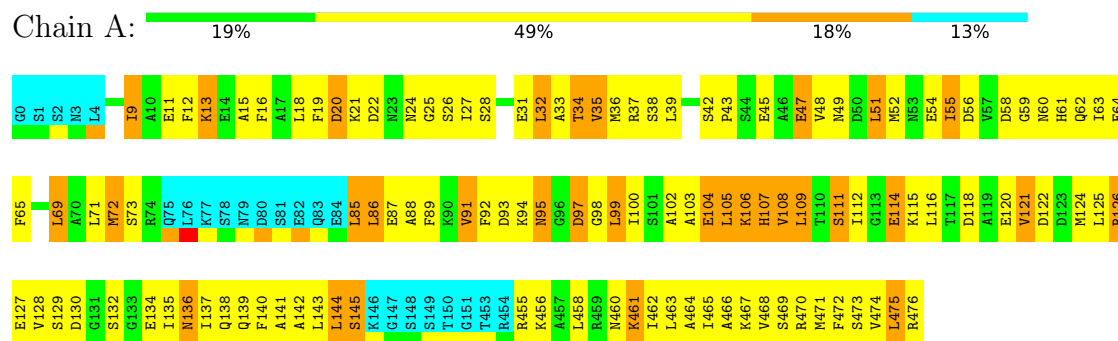
### 4.2.6 Score per residue for model 6

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



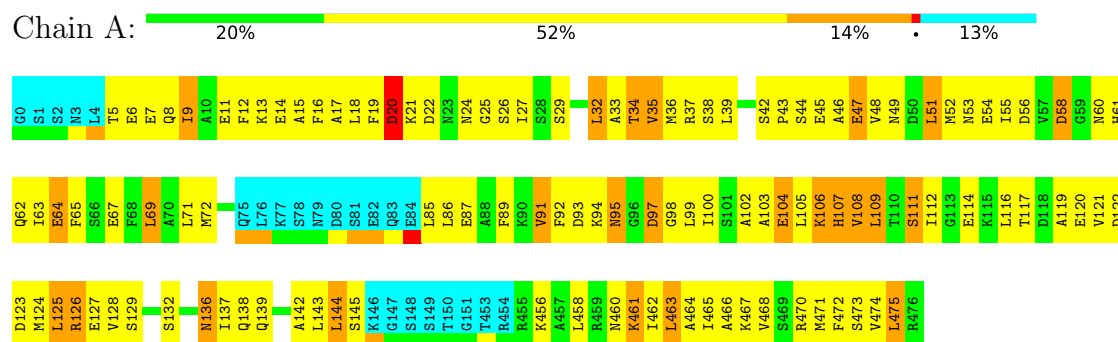
### 4.2.7 Score per residue for model 7

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



### 4.2.8 Score per residue for model 8

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



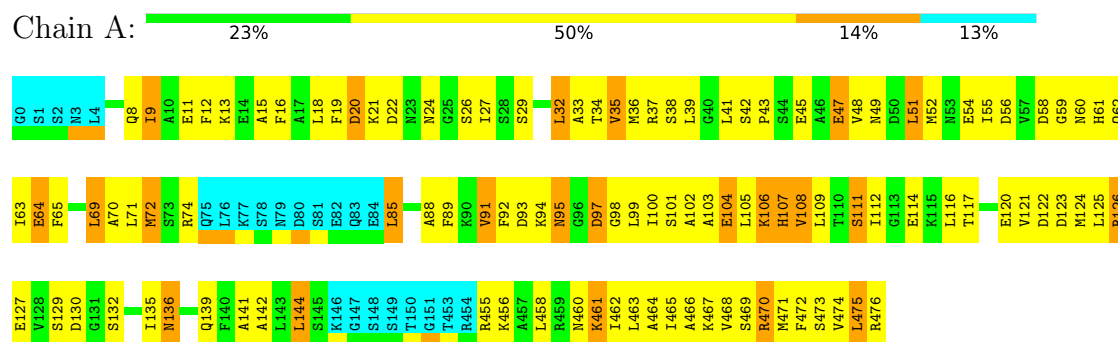
### 4.2.11 Score per residue for model 11

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



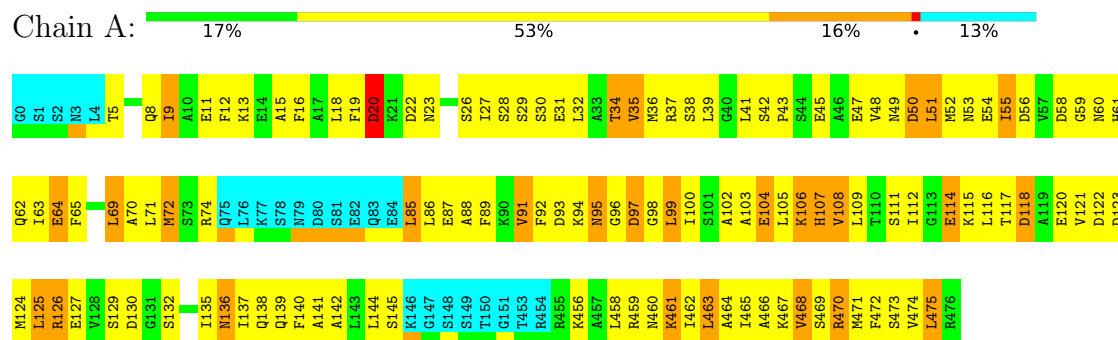
#### 4.2.14 Score per residue for model 14

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



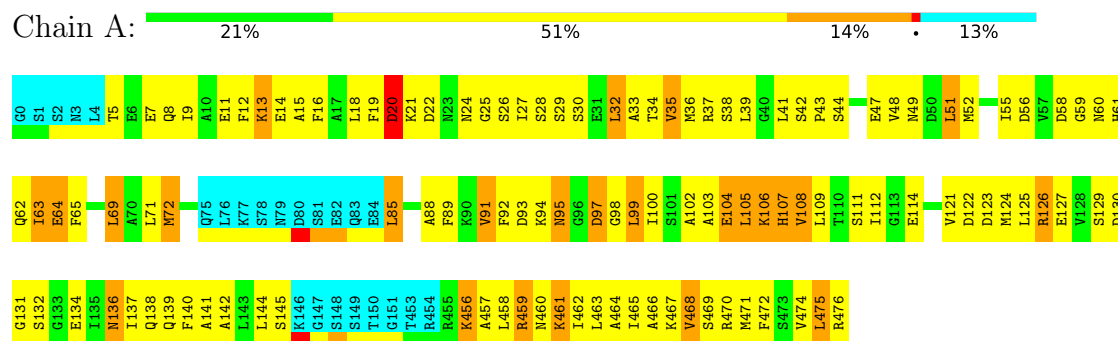
#### 4.2.15 Score per residue for model 15

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



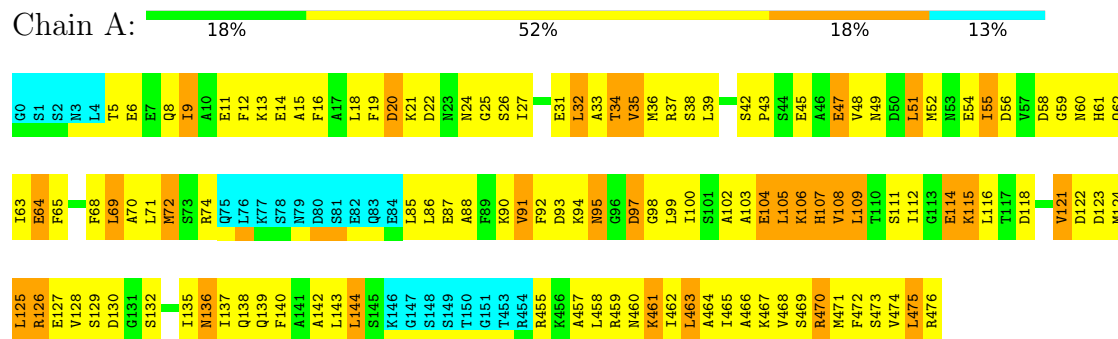
#### 4.2.16 Score per residue for model 16

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



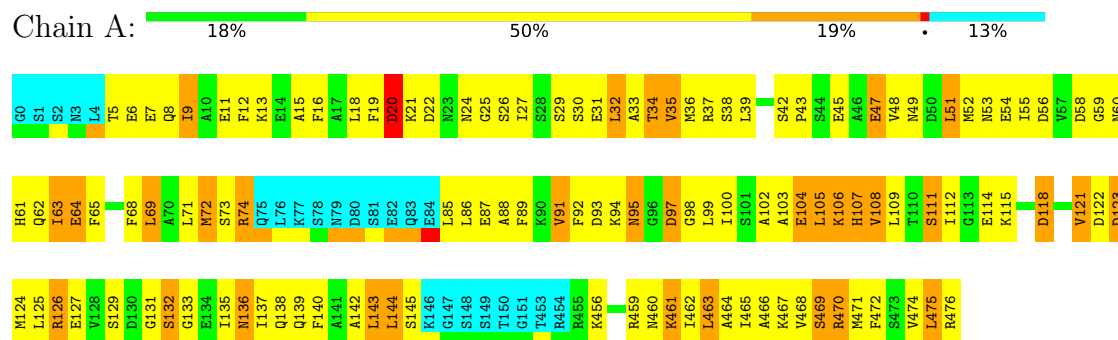
#### 4.2.17 Score per residue for model 17

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



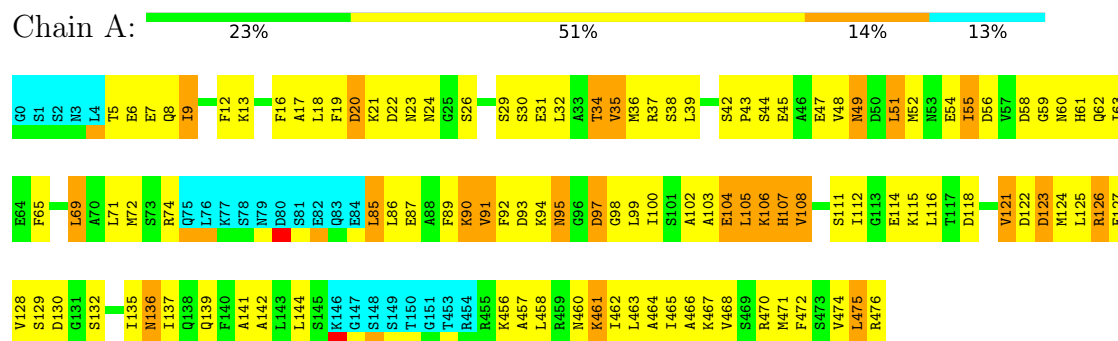
#### 4.2.18 Score per residue for model 18

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



#### 4.2.19 Score per residue for model 19

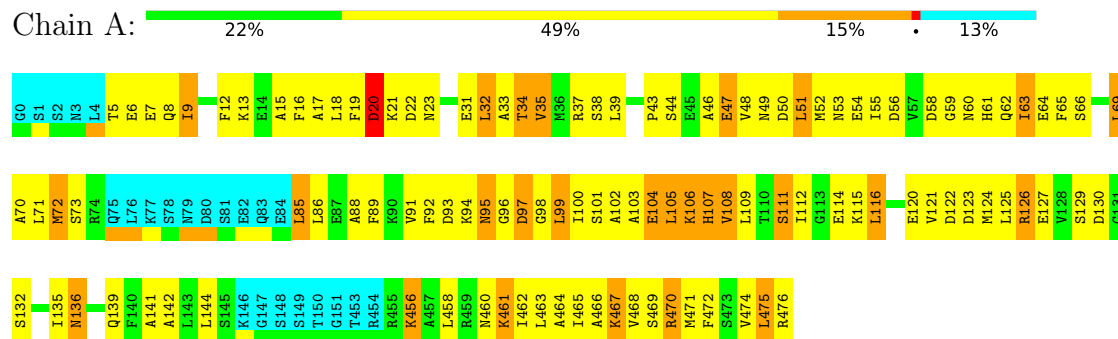
- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1



#### 4.2.20 Score per residue for model 20

- Molecule 1: Calmodulin,Serine/threonine-protein phosphatase 2B catalytic subunit A1

Chain A:



## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification        | Version        |
|---------------|-----------------------|----------------|
| Sparky        | refinement            | 3.113          |
| CYANA         | geometry optimization | 2.1            |
| CYANA         | structure solution    | 2.1            |
| TALOS         | structure solution    | 2003.027.13.05 |

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                       | 2204           |
| Number of shifts mapped to atoms             | 2204           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 94%            |

## 6 Model quality [i](#)

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

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 1182  | 1190     | 1182     | 163±8   |
| All | All   | 23700 | 23800    | 23640    | 3267    |

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 69.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:112:ILE:HG21 | 1:A:465:ILE:HD11 | 1.11     | 1.20        | 16     | 20    |
| 1:A:85:LEU:HD11  | 1:A:141:ALA:HB2  | 1.08     | 1.22        | 12     | 8     |
| 1:A:9:ILE:HG22   | 1:A:65:PHE:CZ    | 1.05     | 1.85        | 12     | 18    |
| 1:A:39:LEU:HD13  | 1:A:465:ILE:HG23 | 1.05     | 1.28        | 14     | 20    |
| 1:A:69:LEU:HD13  | 1:A:70:ALA:N     | 0.99     | 1.73        | 9      | 5     |
| 1:A:85:LEU:HD21  | 1:A:141:ALA:HB2  | 0.98     | 1.05        | 20     | 1     |
| 1:A:85:LEU:HD22  | 1:A:144:LEU:HD12 | 0.97     | 1.33        | 3      | 8     |
| 1:A:85:LEU:HD21  | 1:A:141:ALA:CB   | 0.96     | 1.91        | 20     | 2     |
| 1:A:51:LEU:HD21  | 1:A:471:MET:HE2  | 0.96     | 1.37        | 6      | 2     |
| 1:A:54:GLU:C     | 1:A:55:ILE:HD13  | 0.95     | 1.85        | 10     | 17    |
| 1:A:32:LEU:HD22  | 1:A:48:VAL:HG13  | 0.95     | 1.36        | 16     | 20    |
| 1:A:92:PHE:CZ    | 1:A:108:VAL:HG11 | 0.92     | 1.99        | 18     | 20    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:85:LEU:CD1   | 1:A:141:ALA:HB2  | 0.90     | 1.96        | 12     | 8     |
| 1:A:85:LEU:CD2   | 1:A:141:ALA:HB2  | 0.89     | 1.97        | 20     | 4     |
| 1:A:15:ALA:HB1   | 1:A:464:ALA:HB2  | 0.88     | 1.46        | 2      | 15    |
| 1:A:28:SER:C     | 1:A:52:MET:HE1   | 0.88     | 1.94        | 13     | 10    |
| 1:A:88:ALA:HB2   | 1:A:466:ALA:HB2  | 0.87     | 1.46        | 6      | 17    |
| 1:A:51:LEU:HD21  | 1:A:471:MET:HE3  | 0.87     | 1.45        | 1      | 1     |
| 1:A:114:GLU:OE1  | 1:A:116:LEU:HD13 | 0.87     | 1.69        | 5      | 2     |
| 1:A:125:LEU:HD13 | 1:A:133:GLY:O    | 0.87     | 1.70        | 18     | 3     |
| 1:A:460:ASN:OD1  | 1:A:463:LEU:HD12 | 0.87     | 1.69        | 20     | 1     |
| 1:A:71:LEU:HD21  | 1:A:471:MET:SD   | 0.86     | 2.10        | 9      | 13    |
| 1:A:39:LEU:CD1   | 1:A:465:ILE:HG23 | 0.85     | 2.00        | 5      | 20    |
| 1:A:105:LEU:CD1  | 1:A:135:ILE:HD11 | 0.85     | 2.00        | 20     | 8     |
| 1:A:85:LEU:HD11  | 1:A:141:ALA:CB   | 0.85     | 2.01        | 12     | 7     |
| 1:A:121:VAL:O    | 1:A:125:LEU:HD22 | 0.84     | 1.71        | 8      | 3     |
| 1:A:109:LEU:HD12 | 1:A:116:LEU:HD12 | 0.84     | 1.47        | 10     | 2     |
| 1:A:464:ALA:O    | 1:A:468:VAL:HG22 | 0.83     | 1.73        | 20     | 5     |
| 1:A:112:ILE:HG21 | 1:A:465:ILE:CD1  | 0.82     | 2.04        | 19     | 18    |
| 1:A:112:ILE:CG2  | 1:A:465:ILE:HD11 | 0.82     | 2.04        | 10     | 8     |
| 1:A:98:GLY:O     | 1:A:99:LEU:HD23  | 0.81     | 1.72        | 12     | 17    |
| 1:A:137:ILE:HG23 | 1:A:138:GLN:OE1  | 0.81     | 1.75        | 2      | 2     |
| 1:A:18:LEU:HD21  | 1:A:461:LYS:HG3  | 0.81     | 1.52        | 15     | 11    |
| 1:A:85:LEU:CD2   | 1:A:144:LEU:HD12 | 0.81     | 2.06        | 3      | 5     |
| 1:A:29:SER:N     | 1:A:52:MET:HE1   | 0.78     | 1.94        | 13     | 13    |
| 1:A:19:PHE:CZ    | 1:A:468:VAL:HG11 | 0.78     | 2.13        | 15     | 20    |
| 1:A:69:LEU:HD13  | 1:A:69:LEU:C     | 0.77     | 2.04        | 10     | 5     |
| 1:A:18:LEU:HD21  | 1:A:461:LYS:HG2  | 0.77     | 1.56        | 11     | 8     |
| 1:A:86:LEU:HD12  | 1:A:86:LEU:C     | 0.77     | 2.05        | 4      | 8     |
| 1:A:51:LEU:HD11  | 1:A:471:MET:HE2  | 0.77     | 1.55        | 2      | 5     |
| 1:A:36:MET:HE1   | 1:A:472:PHE:CB   | 0.77     | 2.10        | 3      | 7     |
| 1:A:102:ALA:HA   | 1:A:125:LEU:HD11 | 0.76     | 1.56        | 12     | 3     |
| 1:A:14:GLU:OE2   | 1:A:457:ALA:HB1  | 0.76     | 1.79        | 16     | 1     |
| 1:A:51:LEU:HB2   | 1:A:475:LEU:HD22 | 0.76     | 1.54        | 1      | 7     |
| 1:A:69:LEU:C     | 1:A:69:LEU:HD12  | 0.76     | 2.05        | 2      | 13    |
| 1:A:32:LEU:C     | 1:A:32:LEU:HD23  | 0.75     | 2.06        | 6      | 18    |
| 1:A:92:PHE:CE1   | 1:A:462:ILE:HG23 | 0.75     | 2.16        | 12     | 19    |
| 1:A:51:LEU:C     | 1:A:51:LEU:HD13  | 0.74     | 2.07        | 13     | 13    |
| 1:A:92:PHE:CE2   | 1:A:108:VAL:HG11 | 0.74     | 2.18        | 14     | 20    |
| 1:A:85:LEU:HG    | 1:A:144:LEU:HD12 | 0.74     | 1.59        | 4      | 2     |
| 1:A:105:LEU:HD23 | 1:A:121:VAL:CG2  | 0.73     | 2.13        | 6      | 3     |
| 1:A:461:LYS:O    | 1:A:465:ILE:HD12 | 0.72     | 1.82        | 6      | 13    |
| 1:A:105:LEU:HD11 | 1:A:135:ILE:HD11 | 0.72     | 1.60        | 20     | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:88:ALA:HB2   | 1:A:466:ALA:CB   | 0.72     | 2.15        | 7      | 7     |
| 1:A:110:THR:HG23 | 1:A:115:LYS:HG2  | 0.72     | 1.61        | 10     | 1     |
| 1:A:106:LYS:HG2  | 1:A:121:VAL:HG21 | 0.72     | 1.61        | 8      | 10    |
| 1:A:47:GLU:HB3   | 1:A:475:LEU:HD21 | 0.72     | 1.60        | 18     | 8     |
| 1:A:61:HIS:CG    | 1:A:61:HIS:O     | 0.72     | 2.42        | 5      | 11    |
| 1:A:460:ASN:HA   | 1:A:463:LEU:HD22 | 0.72     | 1.62        | 1      | 6     |
| 1:A:109:LEU:HD13 | 1:A:114:GLU:OE1  | 0.71     | 1.85        | 10     | 1     |
| 1:A:9:ILE:N      | 1:A:9:ILE:HD13   | 0.71     | 2.01        | 5      | 20    |
| 1:A:51:LEU:HD21  | 1:A:471:MET:CE   | 0.71     | 2.16        | 1      | 2     |
| 1:A:105:LEU:HD23 | 1:A:121:VAL:HG23 | 0.70     | 1.63        | 5      | 6     |
| 1:A:18:LEU:HD21  | 1:A:461:LYS:CG   | 0.70     | 2.17        | 17     | 9     |
| 1:A:36:MET:HE1   | 1:A:472:PHE:HB2  | 0.70     | 1.61        | 3      | 9     |
| 1:A:39:LEU:HD23  | 1:A:111:SER:OG   | 0.70     | 1.87        | 2      | 10    |
| 1:A:85:LEU:HG    | 1:A:141:ALA:HB2  | 0.70     | 1.64        | 10     | 3     |
| 1:A:15:ALA:HB1   | 1:A:464:ALA:CB   | 0.70     | 2.15        | 2      | 4     |
| 1:A:55:ILE:HG13  | 1:A:71:LEU:HD22  | 0.70     | 1.64        | 20     | 4     |
| 1:A:9:ILE:HG22   | 1:A:65:PHE:HZ    | 0.70     | 1.47        | 14     | 14    |
| 1:A:51:LEU:HD11  | 1:A:471:MET:HE3  | 0.70     | 1.64        | 17     | 5     |
| 1:A:144:LEU:HD23 | 1:A:144:LEU:N    | 0.69     | 2.02        | 14     | 12    |
| 1:A:55:ILE:HD13  | 1:A:55:ILE:N     | 0.69     | 2.01        | 10     | 4     |
| 1:A:69:LEU:HD12  | 1:A:69:LEU:O     | 0.69     | 1.87        | 7      | 15    |
| 1:A:85:LEU:HB3   | 1:A:137:ILE:HD11 | 0.69     | 1.64        | 5      | 5     |
| 1:A:116:LEU:HD23 | 1:A:120:GLU:HB3  | 0.69     | 1.64        | 1      | 5     |
| 1:A:475:LEU:HD12 | 1:A:475:LEU:O    | 0.68     | 1.88        | 20     | 6     |
| 1:A:102:ALA:HB1  | 1:A:121:VAL:CG1  | 0.68     | 2.19        | 6      | 7     |
| 1:A:51:LEU:C     | 1:A:51:LEU:HD23  | 0.68     | 2.12        | 11     | 3     |
| 1:A:71:LEU:HD21  | 1:A:471:MET:CE   | 0.68     | 2.18        | 18     | 8     |
| 1:A:31:GLU:O     | 1:A:34:THR:HG22  | 0.68     | 1.88        | 18     | 11    |
| 1:A:11:GLU:HB3   | 1:A:456:LYS:HZ3  | 0.68     | 1.48        | 5      | 1     |
| 1:A:47:GLU:CB    | 1:A:475:LEU:HD21 | 0.68     | 2.18        | 6      | 2     |
| 1:A:50:ASP:CG    | 1:A:475:LEU:HD13 | 0.68     | 2.14        | 3      | 1     |
| 1:A:50:ASP:OD1   | 1:A:475:LEU:HD13 | 0.68     | 1.88        | 3      | 1     |
| 1:A:85:LEU:HD22  | 1:A:144:LEU:CD1  | 0.68     | 2.17        | 3      | 2     |
| 1:A:85:LEU:CD1   | 1:A:140:PHE:CD2  | 0.67     | 2.77        | 11     | 4     |
| 1:A:92:PHE:CZ    | 1:A:108:VAL:CG1  | 0.67     | 2.77        | 12     | 20    |
| 1:A:55:ILE:HG21  | 1:A:71:LEU:HB2   | 0.67     | 1.67        | 9      | 7     |
| 1:A:51:LEU:HD11  | 1:A:471:MET:HB3  | 0.67     | 1.66        | 3      | 2     |
| 1:A:36:MET:CE    | 1:A:41:LEU:HD13  | 0.66     | 2.20        | 11     | 6     |
| 1:A:39:LEU:HD13  | 1:A:465:ILE:CG2  | 0.66     | 2.18        | 5      | 6     |
| 1:A:85:LEU:CG    | 1:A:141:ALA:HB2  | 0.66     | 2.21        | 10     | 1     |
| 1:A:99:LEU:HD23  | 1:A:136:ASN:HB3  | 0.66     | 1.67        | 6      | 10    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:139:GLN:O    | 1:A:142:ALA:HB3  | 0.66     | 1.91        | 3      | 19    |
| 1:A:51:LEU:HD21  | 1:A:471:MET:HB3  | 0.66     | 1.65        | 17     | 9     |
| 1:A:61:HIS:CD2   | 1:A:61:HIS:O     | 0.66     | 2.49        | 17     | 8     |
| 1:A:72:MET:HG3   | 1:A:467:LYS:HZ3  | 0.66     | 1.50        | 17     | 2     |
| 1:A:61:HIS:O     | 1:A:61:HIS:CG    | 0.65     | 2.50        | 13     | 8     |
| 1:A:21:LYS:HE3   | 1:A:34:THR:HG21  | 0.65     | 1.68        | 8      | 11    |
| 1:A:112:ILE:HD13 | 1:A:465:ILE:HD11 | 0.65     | 1.66        | 18     | 4     |
| 1:A:72:MET:HE3   | 1:A:467:LYS:HB2  | 0.65     | 1.68        | 9      | 8     |
| 1:A:32:LEU:HD23  | 1:A:33:ALA:N     | 0.65     | 2.06        | 1      | 14    |
| 1:A:61:HIS:O     | 1:A:61:HIS:CD2   | 0.65     | 2.50        | 3      | 11    |
| 1:A:116:LEU:CD1  | 1:A:124:MET:HE1  | 0.65     | 2.22        | 8      | 6     |
| 1:A:55:ILE:HD12  | 1:A:71:LEU:HD13  | 0.65     | 1.68        | 8      | 8     |
| 1:A:32:LEU:HD22  | 1:A:48:VAL:CG1   | 0.65     | 2.19        | 6      | 10    |
| 1:A:36:MET:HE1   | 1:A:472:PHE:CG   | 0.65     | 2.27        | 1      | 9     |
| 1:A:105:LEU:HD21 | 1:A:124:MET:SD   | 0.64     | 2.32        | 8      | 3     |
| 1:A:11:GLU:CB    | 1:A:456:LYS:HZ3  | 0.64     | 2.05        | 5      | 1     |
| 1:A:92:PHE:CZ    | 1:A:462:ILE:HG23 | 0.64     | 2.28        | 12     | 1     |
| 1:A:65:PHE:CD1   | 1:A:65:PHE:O     | 0.64     | 2.51        | 16     | 20    |
| 1:A:36:MET:HE3   | 1:A:41:LEU:HD13  | 0.63     | 1.70        | 11     | 2     |
| 1:A:97:ASP:OD2   | 1:A:99:LEU:HD12  | 0.63     | 1.94        | 6      | 19    |
| 1:A:85:LEU:HD13  | 1:A:140:PHE:CE2  | 0.63     | 2.28        | 11     | 2     |
| 1:A:107:HIS:CD2  | 1:A:108:VAL:HG23 | 0.63     | 2.29        | 12     | 19    |
| 1:A:69:LEU:HD12  | 1:A:69:LEU:C     | 0.63     | 2.19        | 3      | 2     |
| 1:A:21:LYS:CE    | 1:A:34:THR:HG21  | 0.63     | 2.24        | 18     | 5     |
| 1:A:55:ILE:HG21  | 1:A:71:LEU:HD22  | 0.62     | 1.71        | 11     | 2     |
| 1:A:85:LEU:HD21  | 1:A:141:ALA:HA   | 0.62     | 1.69        | 7      | 7     |
| 1:A:116:LEU:HD22 | 1:A:120:GLU:HB3  | 0.62     | 1.72        | 12     | 3     |
| 1:A:459:ARG:O    | 1:A:463:LEU:HD13 | 0.62     | 1.93        | 10     | 5     |
| 1:A:137:ILE:HG23 | 1:A:138:GLN:HE21 | 0.61     | 1.53        | 12     | 5     |
| 1:A:19:PHE:CE2   | 1:A:35:VAL:HG11  | 0.61     | 2.30        | 16     | 3     |
| 1:A:14:GLU:CD    | 1:A:457:ALA:HB1  | 0.61     | 2.20        | 10     | 1     |
| 1:A:19:PHE:CZ    | 1:A:468:VAL:HG21 | 0.61     | 2.30        | 2      | 7     |
| 1:A:19:PHE:CE1   | 1:A:468:VAL:HG11 | 0.61     | 2.30        | 15     | 2     |
| 1:A:69:LEU:HD22  | 1:A:69:LEU:O     | 0.61     | 1.95        | 12     | 5     |
| 1:A:105:LEU:HD12 | 1:A:135:ILE:HD11 | 0.61     | 1.72        | 9      | 5     |
| 1:A:470:ARG:NH1  | 1:A:474:VAL:HG21 | 0.61     | 2.11        | 18     | 1     |
| 1:A:16:PHE:CE2   | 1:A:20:ASP:OD2   | 0.61     | 2.54        | 1      | 19    |
| 1:A:50:ASP:OD2   | 1:A:475:LEU:HD13 | 0.61     | 1.94        | 3      | 1     |
| 1:A:16:PHE:CZ    | 1:A:64:GLU:C     | 0.61     | 2.78        | 17     | 13    |
| 1:A:71:LEU:HD11  | 1:A:471:MET:SD   | 0.61     | 2.35        | 13     | 3     |
| 1:A:71:LEU:HD21  | 1:A:471:MET:HE2  | 0.61     | 1.73        | 4      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:9:ILE:HG23   | 1:A:69:LEU:HD22  | 0.60     | 1.72        | 7      | 6     |
| 1:A:18:LEU:CD2   | 1:A:112:ILE:HD12 | 0.60     | 2.25        | 19     | 10    |
| 1:A:92:PHE:HE2   | 1:A:105:LEU:HD12 | 0.60     | 1.55        | 14     | 2     |
| 1:A:72:MET:HE2   | 1:A:464:ALA:HA   | 0.60     | 1.72        | 16     | 6     |
| 1:A:9:ILE:HG22   | 1:A:65:PHE:CE1   | 0.60     | 2.30        | 20     | 5     |
| 1:A:116:LEU:CD2  | 1:A:124:MET:CE   | 0.60     | 2.79        | 19     | 3     |
| 1:A:72:MET:HE3   | 1:A:467:LYS:HD2  | 0.60     | 1.73        | 15     | 3     |
| 1:A:87:GLU:O     | 1:A:91:VAL:HG23  | 0.60     | 1.96        | 12     | 10    |
| 1:A:14:GLU:HG3   | 1:A:457:ALA:HB1  | 0.60     | 1.73        | 17     | 1     |
| 1:A:92:PHE:CE1   | 1:A:108:VAL:HG11 | 0.60     | 2.32        | 20     | 17    |
| 1:A:109:LEU:HD12 | 1:A:116:LEU:CD1  | 0.60     | 2.26        | 7      | 2     |
| 1:A:475:LEU:HD12 | 1:A:475:LEU:C    | 0.59     | 2.21        | 20     | 2     |
| 1:A:32:LEU:CD2   | 1:A:48:VAL:HG13  | 0.59     | 2.24        | 9      | 5     |
| 1:A:105:LEU:HD22 | 1:A:125:LEU:HD11 | 0.59     | 1.74        | 15     | 2     |
| 1:A:128:VAL:HG11 | 1:A:142:ALA:CB   | 0.59     | 2.28        | 10     | 9     |
| 1:A:92:PHE:CE2   | 1:A:105:LEU:HD12 | 0.59     | 2.32        | 14     | 3     |
| 1:A:92:PHE:CE2   | 1:A:108:VAL:CG1  | 0.59     | 2.86        | 10     | 15    |
| 1:A:137:ILE:HG23 | 1:A:138:GLN:NE2  | 0.59     | 2.11        | 12     | 5     |
| 1:A:13:LYS:CG    | 1:A:65:PHE:CE1   | 0.59     | 2.85        | 1      | 9     |
| 1:A:135:ILE:CD1  | 1:A:143:LEU:HD11 | 0.59     | 2.28        | 7      | 2     |
| 1:A:55:ILE:HD11  | 1:A:471:MET:SD   | 0.59     | 2.38        | 19     | 3     |
| 1:A:114:GLU:HG3  | 1:A:461:LYS:HZ2  | 0.58     | 1.56        | 14     | 1     |
| 1:A:106:LYS:HB3  | 1:A:121:VAL:HG21 | 0.58     | 1.73        | 17     | 8     |
| 1:A:52:MET:HE2   | 1:A:62:GLN:HA    | 0.58     | 1.75        | 20     | 6     |
| 1:A:72:MET:CG    | 1:A:467:LYS:HZ3  | 0.58     | 2.11        | 17     | 1     |
| 1:A:107:HIS:CD2  | 1:A:108:VAL:N    | 0.58     | 2.72        | 14     | 20    |
| 1:A:122:ASP:HA   | 1:A:125:LEU:HD12 | 0.58     | 1.75        | 13     | 2     |
| 1:A:16:PHE:CZ    | 1:A:20:ASP:OD2   | 0.58     | 2.57        | 17     | 2     |
| 1:A:72:MET:HE3   | 1:A:467:LYS:HE2  | 0.58     | 1.74        | 1      | 1     |
| 1:A:99:LEU:HD22  | 1:A:136:ASN:OD1  | 0.57     | 2.00        | 20     | 4     |
| 1:A:51:LEU:C     | 1:A:51:LEU:CD2   | 0.57     | 2.78        | 11     | 6     |
| 1:A:85:LEU:CD2   | 1:A:141:ALA:CB   | 0.57     | 2.83        | 4      | 2     |
| 1:A:50:ASP:HB3   | 1:A:475:LEU:HD13 | 0.57     | 1.74        | 11     | 2     |
| 1:A:116:LEU:CD2  | 1:A:124:MET:HE3  | 0.57     | 2.28        | 17     | 1     |
| 1:A:456:LYS:HE3  | 1:A:457:ALA:HB2  | 0.57     | 1.77        | 5      | 1     |
| 1:A:51:LEU:CD2   | 1:A:471:MET:HE2  | 0.57     | 2.26        | 11     | 1     |
| 1:A:15:ALA:O     | 1:A:68:PHE:CZ    | 0.57     | 2.58        | 17     | 5     |
| 1:A:86:LEU:HD12  | 1:A:87:GLU:N     | 0.57     | 2.14        | 19     | 7     |
| 1:A:105:LEU:HD13 | 1:A:135:ILE:HD11 | 0.57     | 1.75        | 6      | 4     |
| 1:A:92:PHE:CB    | 1:A:100:ILE:HD13 | 0.56     | 2.29        | 8      | 19    |
| 1:A:92:PHE:HE1   | 1:A:462:ILE:HG23 | 0.56     | 1.58        | 10     | 17    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:51:LEU:C     | 1:A:51:LEU:CD1   | 0.56     | 2.78        | 16     | 14    |
| 1:A:85:LEU:HD11  | 1:A:141:ALA:CA   | 0.56     | 2.31        | 10     | 11    |
| 1:A:72:MET:HE3   | 1:A:467:LYS:CB   | 0.56     | 2.30        | 2      | 5     |
| 1:A:85:LEU:HD13  | 1:A:140:PHE:CD2  | 0.56     | 2.36        | 11     | 4     |
| 1:A:71:LEU:CD2   | 1:A:471:MET:HE2  | 0.56     | 2.30        | 4      | 1     |
| 1:A:19:PHE:CE2   | 1:A:35:VAL:CG1   | 0.56     | 2.89        | 16     | 3     |
| 1:A:124:MET:CE   | 1:A:458:LEU:HD11 | 0.56     | 2.31        | 12     | 1     |
| 1:A:15:ALA:N     | 1:A:461:LYS:HZ1  | 0.55     | 2.00        | 4      | 1     |
| 1:A:109:LEU:HD11 | 1:A:458:LEU:HD11 | 0.55     | 1.79        | 13     | 1     |
| 1:A:58:ASP:OD1   | 1:A:58:ASP:C     | 0.55     | 2.49        | 16     | 19    |
| 1:A:58:ASP:OD1   | 1:A:58:ASP:N     | 0.55     | 2.40        | 8      | 1     |
| 1:A:55:ILE:HD12  | 1:A:71:LEU:CD1   | 0.55     | 2.32        | 2      | 4     |
| 1:A:51:LEU:HD13  | 1:A:51:LEU:O     | 0.55     | 2.02        | 18     | 8     |
| 1:A:107:HIS:NE2  | 1:A:108:VAL:HG23 | 0.55     | 2.16        | 10     | 13    |
| 1:A:18:LEU:CD1   | 1:A:464:ALA:HB3  | 0.55     | 2.32        | 1      | 7     |
| 1:A:86:LEU:C     | 1:A:86:LEU:CD1   | 0.54     | 2.80        | 7      | 3     |
| 1:A:32:LEU:C     | 1:A:32:LEU:CD2   | 0.54     | 2.80        | 1      | 10    |
| 1:A:41:LEU:HD11  | 1:A:469:SER:OG   | 0.54     | 2.03        | 6      | 1     |
| 1:A:52:MET:HE2   | 1:A:61:HIS:C     | 0.54     | 2.27        | 12     | 2     |
| 1:A:9:ILE:HG23   | 1:A:69:LEU:CD2   | 0.54     | 2.32        | 7      | 3     |
| 1:A:139:GLN:O    | 1:A:142:ALA:CB   | 0.54     | 2.56        | 3      | 17    |
| 1:A:49:ASN:OD1   | 1:A:61:HIS:CE1   | 0.54     | 2.61        | 12     | 2     |
| 1:A:47:GLU:HB3   | 1:A:475:LEU:HD11 | 0.54     | 1.79        | 6      | 1     |
| 1:A:54:GLU:O     | 1:A:55:ILE:HD13  | 0.54     | 2.03        | 17     | 6     |
| 1:A:72:MET:CB    | 1:A:467:LYS:HZ3  | 0.54     | 2.16        | 17     | 1     |
| 1:A:85:LEU:O     | 1:A:89:PHE:N     | 0.54     | 2.41        | 10     | 16    |
| 1:A:69:LEU:C     | 1:A:69:LEU:CD1   | 0.54     | 2.80        | 20     | 16    |
| 1:A:51:LEU:HD12  | 1:A:472:PHE:HA   | 0.54     | 1.78        | 11     | 1     |
| 1:A:55:ILE:HD12  | 1:A:71:LEU:HD12  | 0.54     | 1.80        | 7      | 3     |
| 1:A:33:ALA:HB1   | 1:A:37:ARG:NH2   | 0.54     | 2.17        | 18     | 1     |
| 1:A:112:ILE:HD11 | 1:A:461:LYS:HG2  | 0.53     | 1.79        | 4      | 1     |
| 1:A:51:LEU:HD21  | 1:A:471:MET:C    | 0.53     | 2.28        | 10     | 4     |
| 1:A:19:PHE:CD1   | 1:A:27:ILE:HD13  | 0.53     | 2.38        | 12     | 2     |
| 1:A:51:LEU:C     | 1:A:51:LEU:HD22  | 0.53     | 2.28        | 4      | 3     |
| 1:A:11:GLU:CD    | 1:A:456:LYS:CD   | 0.53     | 2.81        | 18     | 2     |
| 1:A:66:SER:O     | 1:A:69:LEU:CD1   | 0.53     | 2.56        | 9      | 5     |
| 1:A:87:GLU:O     | 1:A:91:VAL:CG2   | 0.53     | 2.56        | 19     | 11    |
| 1:A:109:LEU:HD12 | 1:A:114:GLU:CB   | 0.53     | 2.33        | 4      | 4     |
| 1:A:32:LEU:HD11  | 1:A:51:LEU:HD12  | 0.53     | 1.80        | 5      | 4     |
| 1:A:102:ALA:HB1  | 1:A:121:VAL:HG11 | 0.53     | 1.80        | 6      | 4     |
| 1:A:470:ARG:CD   | 1:A:474:VAL:CG2  | 0.53     | 2.86        | 15     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:112:ILE:CD1  | 1:A:461:LYS:CG   | 0.53     | 2.87        | 12     | 7     |
| 1:A:58:ASP:OD1   | 1:A:59:GLY:N     | 0.53     | 2.41        | 19     | 19    |
| 1:A:13:LYS:HG3   | 1:A:65:PHE:CE1   | 0.53     | 2.39        | 1      | 8     |
| 1:A:61:HIS:O     | 1:A:62:GLN:CG    | 0.53     | 2.57        | 18     | 11    |
| 1:A:70:ALA:O     | 1:A:74:ARG:CB    | 0.53     | 2.57        | 15     | 5     |
| 1:A:121:VAL:CG1  | 1:A:122:ASP:N    | 0.53     | 2.72        | 19     | 19    |
| 1:A:105:LEU:CD1  | 1:A:135:ILE:CD1  | 0.53     | 2.85        | 3      | 4     |
| 1:A:140:PHE:CZ   | 1:A:144:LEU:HD11 | 0.53     | 2.39        | 15     | 1     |
| 1:A:456:LYS:CB   | 1:A:459:ARG:NH2  | 0.53     | 2.72        | 9      | 2     |
| 1:A:91:VAL:CG1   | 1:A:92:PHE:N     | 0.52     | 2.72        | 14     | 7     |
| 1:A:13:LYS:HG2   | 1:A:65:PHE:CE1   | 0.52     | 2.39        | 19     | 7     |
| 1:A:8:GLN:O      | 1:A:12:PHE:CD2   | 0.52     | 2.63        | 4      | 5     |
| 1:A:102:ALA:HB1  | 1:A:121:VAL:HG13 | 0.52     | 1.81        | 8      | 1     |
| 1:A:43:PRO:HA    | 1:A:472:PHE:CZ   | 0.52     | 2.40        | 6      | 1     |
| 1:A:18:LEU:HD22  | 1:A:112:ILE:HB   | 0.52     | 1.80        | 8      | 6     |
| 1:A:99:LEU:HD23  | 1:A:136:ASN:CB   | 0.52     | 2.34        | 9      | 3     |
| 1:A:19:PHE:HB2   | 1:A:27:ILE:HD13  | 0.52     | 1.82        | 18     | 11    |
| 1:A:92:PHE:CD2   | 1:A:105:LEU:HD22 | 0.52     | 2.40        | 1      | 1     |
| 1:A:13:LYS:HG3   | 1:A:65:PHE:CZ    | 0.52     | 2.40        | 19     | 11    |
| 1:A:114:GLU:CD   | 1:A:115:LYS:N    | 0.52     | 2.68        | 12     | 4     |
| 1:A:36:MET:SD    | 1:A:41:LEU:HD13  | 0.52     | 2.45        | 16     | 3     |
| 1:A:135:ILE:HD12 | 1:A:143:LEU:HD11 | 0.52     | 1.80        | 7      | 2     |
| 1:A:52:MET:HE2   | 1:A:61:HIS:O     | 0.52     | 2.04        | 12     | 4     |
| 1:A:463:LEU:O    | 1:A:466:ALA:HB3  | 0.52     | 2.05        | 12     | 2     |
| 1:A:95:ASN:ND2   | 1:A:95:ASN:C     | 0.52     | 2.68        | 1      | 16    |
| 1:A:116:LEU:HD13 | 1:A:120:GLU:HB3  | 0.52     | 1.83        | 13     | 2     |
| 1:A:124:MET:O    | 1:A:127:GLU:CG   | 0.51     | 2.59        | 11     | 9     |
| 1:A:16:PHE:CZ    | 1:A:65:PHE:N     | 0.51     | 2.78        | 3      | 7     |
| 1:A:470:ARG:O    | 1:A:473:SER:N    | 0.51     | 2.43        | 14     | 10    |
| 1:A:128:VAL:HG11 | 1:A:142:ALA:HB1  | 0.51     | 1.80        | 10     | 2     |
| 1:A:51:LEU:CD1   | 1:A:471:MET:HE2  | 0.51     | 2.34        | 20     | 1     |
| 1:A:19:PHE:CE2   | 1:A:35:VAL:HB    | 0.51     | 2.40        | 17     | 9     |
| 1:A:105:LEU:HD22 | 1:A:125:LEU:CD1  | 0.51     | 2.35        | 15     | 2     |
| 1:A:85:LEU:HD12  | 1:A:137:ILE:HD12 | 0.51     | 1.81        | 9      | 5     |
| 1:A:13:LYS:HA    | 1:A:65:PHE:CE1   | 0.51     | 2.41        | 16     | 1     |
| 1:A:31:GLU:O     | 1:A:34:THR:CG2   | 0.51     | 2.59        | 1      | 11    |
| 1:A:51:LEU:O     | 1:A:51:LEU:HD13  | 0.51     | 2.05        | 8      | 3     |
| 1:A:103:ALA:O    | 1:A:107:HIS:N    | 0.51     | 2.44        | 6      | 17    |
| 1:A:106:LYS:O    | 1:A:109:LEU:N    | 0.51     | 2.44        | 14     | 10    |
| 1:A:121:VAL:HG13 | 1:A:122:ASP:N    | 0.51     | 2.21        | 15     | 13    |
| 1:A:29:SER:O     | 1:A:48:VAL:HG11  | 0.51     | 2.05        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:120:GLU:CD   | 1:A:120:GLU:N    | 0.51     | 2.69        | 2      | 1     |
| 1:A:118:ASP:O    | 1:A:122:ASP:CB   | 0.51     | 2.59        | 7      | 6     |
| 1:A:103:ALA:C    | 1:A:105:LEU:N    | 0.51     | 2.67        | 19     | 20    |
| 1:A:18:LEU:O     | 1:A:35:VAL:CG2   | 0.50     | 2.60        | 6      | 14    |
| 1:A:50:ASP:OD2   | 1:A:475:LEU:CD1  | 0.50     | 2.58        | 3      | 1     |
| 1:A:106:LYS:CB   | 1:A:121:VAL:HG21 | 0.50     | 2.36        | 5      | 3     |
| 1:A:99:LEU:CD2   | 1:A:136:ASN:OD1  | 0.50     | 2.59        | 19     | 5     |
| 1:A:105:LEU:HD23 | 1:A:135:ILE:HD11 | 0.50     | 1.82        | 12     | 1     |
| 1:A:51:LEU:HD23  | 1:A:472:PHE:HA   | 0.50     | 1.83        | 15     | 1     |
| 1:A:43:PRO:HB3   | 1:A:472:PHE:CE1  | 0.50     | 2.42        | 6      | 13    |
| 1:A:106:LYS:CG   | 1:A:121:VAL:HG21 | 0.50     | 2.35        | 15     | 5     |
| 1:A:125:LEU:C    | 1:A:127:GLU:N    | 0.50     | 2.69        | 4      | 20    |
| 1:A:139:GLN:O    | 1:A:142:ALA:N    | 0.50     | 2.44        | 18     | 20    |
| 1:A:125:LEU:O    | 1:A:129:SER:N    | 0.50     | 2.44        | 5      | 19    |
| 1:A:466:ALA:O    | 1:A:467:LYS:C    | 0.50     | 2.55        | 2      | 5     |
| 1:A:467:LYS:C    | 1:A:469:SER:N    | 0.50     | 2.69        | 16     | 12    |
| 1:A:114:GLU:CG   | 1:A:461:LYS:HZ2  | 0.50     | 2.20        | 14     | 1     |
| 1:A:13:LYS:CB    | 1:A:65:PHE:CZ    | 0.50     | 2.94        | 16     | 1     |
| 1:A:56:ASP:OD2   | 1:A:60:ASN:N     | 0.50     | 2.44        | 18     | 15    |
| 1:A:125:LEU:O    | 1:A:127:GLU:N    | 0.50     | 2.45        | 18     | 20    |
| 1:A:19:PHE:CE1   | 1:A:35:VAL:HB    | 0.50     | 2.42        | 15     | 11    |
| 1:A:29:SER:OG    | 1:A:48:VAL:CG1   | 0.50     | 2.60        | 14     | 4     |
| 1:A:52:MET:HB2   | 1:A:63:ILE:HD11  | 0.50     | 1.84        | 2      | 4     |
| 1:A:112:ILE:CD1  | 1:A:461:LYS:CD   | 0.50     | 2.90        | 10     | 2     |
| 1:A:109:LEU:O    | 1:A:112:ILE:CG1  | 0.50     | 2.60        | 12     | 7     |
| 1:A:103:ALA:O    | 1:A:105:LEU:N    | 0.50     | 2.44        | 19     | 20    |
| 1:A:19:PHE:HZ    | 1:A:468:VAL:HG11 | 0.50     | 1.61        | 6      | 7     |
| 1:A:19:PHE:CD2   | 1:A:35:VAL:HB    | 0.50     | 2.42        | 16     | 9     |
| 1:A:71:LEU:CD2   | 1:A:471:MET:SD   | 0.50     | 2.99        | 13     | 3     |
| 1:A:9:ILE:CG2    | 1:A:65:PHE:CZ    | 0.49     | 2.79        | 12     | 6     |
| 1:A:470:ARG:HH11 | 1:A:474:VAL:HG21 | 0.49     | 1.66        | 18     | 1     |
| 1:A:125:LEU:O    | 1:A:126:ARG:C    | 0.49     | 2.55        | 8      | 20    |
| 1:A:72:MET:HE2   | 1:A:467:LYS:HD3  | 0.49     | 1.84        | 4      | 1     |
| 1:A:19:PHE:CD1   | 1:A:35:VAL:HB    | 0.49     | 2.43        | 10     | 11    |
| 1:A:9:ILE:HG23   | 1:A:69:LEU:HG    | 0.49     | 1.84        | 20     | 2     |
| 1:A:98:GLY:O     | 1:A:99:LEU:CD2   | 0.49     | 2.59        | 14     | 15    |
| 1:A:39:LEU:CD2   | 1:A:111:SER:OG   | 0.49     | 2.60        | 10     | 9     |
| 1:A:74:ARG:CG    | 1:A:74:ARG:O     | 0.49     | 2.60        | 15     | 6     |
| 1:A:456:LYS:NZ   | 1:A:460:ASN:ND2  | 0.49     | 2.60        | 20     | 1     |
| 1:A:467:LYS:O    | 1:A:470:ARG:N    | 0.49     | 2.46        | 10     | 10    |
| 1:A:141:ALA:O    | 1:A:145:SER:N    | 0.49     | 2.46        | 13     | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:37:ARG:CG    | 1:A:38:SER:N     | 0.49     | 2.75        | 5      | 13    |
| 1:A:47:GLU:C     | 1:A:49:ASN:N     | 0.49     | 2.69        | 4      | 13    |
| 1:A:52:MET:CB    | 1:A:63:ILE:HD11  | 0.49     | 2.38        | 2      | 5     |
| 1:A:72:MET:HE1   | 1:A:467:LYS:HB2  | 0.49     | 1.84        | 3      | 1     |
| 1:A:72:MET:SD    | 1:A:72:MET:N     | 0.49     | 2.85        | 6      | 9     |
| 1:A:102:ALA:O    | 1:A:105:LEU:N    | 0.49     | 2.45        | 11     | 19    |
| 1:A:116:LEU:HD13 | 1:A:124:MET:CE   | 0.49     | 2.38        | 8      | 2     |
| 1:A:97:ASP:OD1   | 1:A:99:LEU:N     | 0.49     | 2.45        | 7      | 19    |
| 1:A:136:ASN:C    | 1:A:138:GLN:N    | 0.49     | 2.69        | 13     | 13    |
| 1:A:51:LEU:CD2   | 1:A:471:MET:O    | 0.49     | 2.61        | 9      | 3     |
| 1:A:56:ASP:OD2   | 1:A:61:HIS:N     | 0.48     | 2.46        | 10     | 5     |
| 1:A:105:LEU:HD13 | 1:A:109:LEU:HD23 | 0.48     | 1.84        | 12     | 1     |
| 1:A:43:PRO:HB3   | 1:A:472:PHE:CZ   | 0.48     | 2.44        | 5      | 6     |
| 1:A:27:ILE:O     | 1:A:52:MET:HE1   | 0.48     | 2.07        | 8      | 3     |
| 1:A:69:LEU:C     | 1:A:69:LEU:HD22  | 0.48     | 2.33        | 9      | 4     |
| 1:A:132:SER:OG   | 1:A:133:GLY:N    | 0.48     | 2.46        | 9      | 2     |
| 1:A:458:LEU:HD22 | 1:A:461:LYS:NZ   | 0.48     | 2.23        | 13     | 1     |
| 1:A:114:GLU:CG   | 1:A:461:LYS:NZ   | 0.48     | 2.76        | 14     | 1     |
| 1:A:55:ILE:O     | 1:A:56:ASP:C     | 0.48     | 2.56        | 12     | 20    |
| 1:A:27:ILE:O     | 1:A:52:MET:CE    | 0.48     | 2.62        | 16     | 3     |
| 1:A:127:GLU:OE1  | 1:A:455:ARG:CZ   | 0.48     | 2.61        | 2      | 1     |
| 1:A:9:ILE:N      | 1:A:9:ILE:CD1    | 0.48     | 2.71        | 3      | 7     |
| 1:A:88:ALA:CB    | 1:A:466:ALA:HB2  | 0.48     | 2.36        | 7      | 1     |
| 1:A:144:LEU:N    | 1:A:144:LEU:CD2  | 0.48     | 2.73        | 14     | 7     |
| 1:A:11:GLU:O     | 1:A:460:ASN:ND2  | 0.48     | 2.47        | 16     | 14    |
| 1:A:469:SER:O    | 1:A:470:ARG:C    | 0.48     | 2.56        | 2      | 4     |
| 1:A:19:PHE:CE2   | 1:A:35:VAL:CB    | 0.48     | 2.96        | 16     | 4     |
| 1:A:51:LEU:HD11  | 1:A:471:MET:CE   | 0.48     | 2.37        | 17     | 2     |
| 1:A:129:SER:O    | 1:A:130:ASP:C    | 0.48     | 2.57        | 1      | 15    |
| 1:A:474:VAL:O    | 1:A:475:LEU:C    | 0.48     | 2.57        | 1      | 19    |
| 1:A:114:GLU:O    | 1:A:114:GLU:CG   | 0.48     | 2.61        | 10     | 1     |
| 1:A:105:LEU:HD13 | 1:A:125:LEU:CD1  | 0.48     | 2.39        | 17     | 1     |
| 1:A:45:GLU:O     | 1:A:49:ASN:ND2   | 0.48     | 2.47        | 19     | 14    |
| 1:A:464:ALA:C    | 1:A:466:ALA:N    | 0.48     | 2.71        | 14     | 19    |
| 1:A:13:LYS:HE2   | 1:A:65:PHE:CE2   | 0.48     | 2.44        | 5      | 2     |
| 1:A:142:ALA:O    | 1:A:145:SER:C    | 0.48     | 2.57        | 10     | 6     |
| 1:A:102:ALA:CA   | 1:A:125:LEU:HD11 | 0.48     | 2.35        | 12     | 1     |
| 1:A:66:SER:C     | 1:A:69:LEU:HD12  | 0.48     | 2.34        | 9      | 5     |
| 1:A:456:LYS:HB2  | 1:A:459:ARG:HH21 | 0.48     | 1.69        | 16     | 1     |
| 1:A:129:SER:O    | 1:A:132:SER:N    | 0.47     | 2.47        | 19     | 17    |
| 1:A:13:LYS:CG    | 1:A:65:PHE:CZ    | 0.47     | 2.97        | 19     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:129:SER:C    | 1:A:131:GLY:N    | 0.47     | 2.71        | 16     | 2     |
| 1:A:128:VAL:CG2  | 1:A:143:LEU:CD1  | 0.47     | 2.92        | 13     | 1     |
| 1:A:474:VAL:C    | 1:A:476:ARG:N    | 0.47     | 2.70        | 14     | 10    |
| 1:A:89:PHE:CE1   | 1:A:137:ILE:N    | 0.47     | 2.81        | 12     | 4     |
| 1:A:144:LEU:HD21 | 1:A:462:ILE:HD12 | 0.47     | 1.85        | 19     | 1     |
| 1:A:56:ASP:OD1   | 1:A:58:ASP:OD1   | 0.47     | 2.33        | 20     | 20    |
| 1:A:33:ALA:HB2   | 1:A:48:VAL:HG21  | 0.47     | 1.85        | 9      | 7     |
| 1:A:459:ARG:CG   | 1:A:460:ASN:N    | 0.47     | 2.76        | 13     | 3     |
| 1:A:31:GLU:O     | 1:A:34:THR:CB    | 0.47     | 2.61        | 20     | 4     |
| 1:A:36:MET:SD    | 1:A:41:LEU:CD1   | 0.47     | 3.02        | 16     | 2     |
| 1:A:143:LEU:O    | 1:A:459:ARG:NH1  | 0.47     | 2.48        | 11     | 3     |
| 1:A:466:ALA:O    | 1:A:469:SER:N    | 0.47     | 2.48        | 2      | 5     |
| 1:A:50:ASP:OD1   | 1:A:51:LEU:N     | 0.47     | 2.48        | 3      | 1     |
| 1:A:105:LEU:C    | 1:A:105:LEU:CD1  | 0.47     | 2.87        | 12     | 1     |
| 1:A:127:GLU:CD   | 1:A:455:ARG:NH1  | 0.47     | 2.73        | 2      | 1     |
| 1:A:467:LYS:O    | 1:A:468:VAL:C    | 0.47     | 2.58        | 16     | 16    |
| 1:A:95:ASN:OD1   | 1:A:96:GLY:N     | 0.47     | 2.47        | 6      | 4     |
| 1:A:16:PHE:CE2   | 1:A:65:PHE:HB2   | 0.47     | 2.43        | 16     | 1     |
| 1:A:19:PHE:HZ    | 1:A:468:VAL:HG21 | 0.47     | 1.70        | 13     | 5     |
| 1:A:13:LYS:HB2   | 1:A:65:PHE:CZ    | 0.47     | 2.45        | 16     | 1     |
| 1:A:49:ASN:HD22  | 1:A:49:ASN:N     | 0.47     | 2.08        | 19     | 1     |
| 1:A:49:ASN:C     | 1:A:51:LEU:N     | 0.47     | 2.72        | 3      | 11    |
| 1:A:61:HIS:C     | 1:A:62:GLN:CG    | 0.47     | 2.88        | 6      | 7     |
| 1:A:52:MET:SD    | 1:A:61:HIS:C     | 0.47     | 2.98        | 19     | 4     |
| 1:A:11:GLU:OE1   | 1:A:456:LYS:CG   | 0.47     | 2.63        | 18     | 1     |
| 1:A:109:LEU:C    | 1:A:114:GLU:O    | 0.47     | 2.58        | 10     | 7     |
| 1:A:135:ILE:HD12 | 1:A:143:LEU:CD1  | 0.47     | 2.40        | 7      | 1     |
| 1:A:144:LEU:HD13 | 1:A:463:LEU:CD1  | 0.47     | 2.39        | 17     | 1     |
| 1:A:461:LYS:HZ3  | 1:A:461:LYS:N    | 0.47     | 2.07        | 19     | 1     |
| 1:A:103:ALA:O    | 1:A:104:GLU:C    | 0.47     | 2.58        | 19     | 20    |
| 1:A:143:LEU:C    | 1:A:459:ARG:NH1  | 0.47     | 2.73        | 1      | 1     |
| 1:A:49:ASN:O     | 1:A:53:ASN:N     | 0.47     | 2.48        | 2      | 9     |
| 1:A:114:GLU:OE2  | 1:A:116:LEU:N    | 0.47     | 2.48        | 5      | 1     |
| 1:A:109:LEU:O    | 1:A:114:GLU:N    | 0.46     | 2.48        | 4      | 6     |
| 1:A:105:LEU:O    | 1:A:108:VAL:N    | 0.46     | 2.48        | 9      | 1     |
| 1:A:472:PHE:CD1  | 1:A:475:LEU:HD23 | 0.46     | 2.45        | 14     | 1     |
| 1:A:464:ALA:O    | 1:A:465:ILE:C    | 0.46     | 2.58        | 9      | 10    |
| 1:A:72:MET:SD    | 1:A:467:LYS:CD   | 0.46     | 3.03        | 5      | 2     |
| 1:A:18:LEU:HD22  | 1:A:112:ILE:HD12 | 0.46     | 1.85        | 4      | 2     |
| 1:A:8:GLN:O      | 1:A:12:PHE:CE2   | 0.46     | 2.68        | 5      | 1     |
| 1:A:106:LYS:HD2  | 1:A:121:VAL:HG11 | 0.46     | 1.86        | 11     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:71:LEU:CD1  | 1:A:471:MET:SD   | 0.46     | 3.03        | 13     | 1     |
| 1:A:461:LYS:N   | 1:A:461:LYS:NZ   | 0.46     | 2.62        | 19     | 1     |
| 1:A:42:SER:N    | 1:A:43:PRO:HD3   | 0.46     | 2.24        | 5      | 19    |
| 1:A:121:VAL:O   | 1:A:124:MET:N    | 0.46     | 2.49        | 8      | 14    |
| 1:A:141:ALA:O   | 1:A:144:LEU:N    | 0.46     | 2.49        | 13     | 2     |
| 1:A:56:ASP:OD1  | 1:A:62:GLN:O     | 0.46     | 2.34        | 14     | 20    |
| 1:A:121:VAL:C   | 1:A:123:ASP:N    | 0.46     | 2.73        | 16     | 15    |
| 1:A:460:ASN:HA  | 1:A:463:LEU:HD12 | 0.46     | 1.88        | 7      | 8     |
| 1:A:21:LYS:CE   | 1:A:34:THR:CG2   | 0.46     | 2.93        | 18     | 2     |
| 1:A:106:LYS:CG  | 1:A:121:VAL:HG11 | 0.46     | 2.40        | 5      | 1     |
| 1:A:14:GLU:CD   | 1:A:457:ALA:CB   | 0.46     | 2.88        | 10     | 1     |
| 1:A:22:ASP:C    | 1:A:22:ASP:OD1   | 0.46     | 2.59        | 20     | 3     |
| 1:A:19:PHE:O    | 1:A:21:LYS:N     | 0.46     | 2.49        | 8      | 15    |
| 1:A:136:ASN:O   | 1:A:140:PHE:N    | 0.46     | 2.47        | 13     | 8     |
| 1:A:467:LYS:O   | 1:A:469:SER:N    | 0.46     | 2.49        | 9      | 7     |
| 1:A:469:SER:C   | 1:A:471:MET:N    | 0.46     | 2.72        | 20     | 2     |
| 1:A:13:LYS:HG3  | 1:A:14:GLU:N     | 0.46     | 2.25        | 16     | 1     |
| 1:A:125:LEU:C   | 1:A:129:SER:OG   | 0.46     | 2.58        | 5      | 2     |
| 1:A:12:PHE:O    | 1:A:15:ALA:N     | 0.46     | 2.49        | 16     | 1     |
| 1:A:85:LEU:HD12 | 1:A:137:ILE:CD1  | 0.46     | 2.41        | 2      | 3     |
| 1:A:141:ALA:C   | 1:A:143:LEU:N    | 0.46     | 2.73        | 13     | 1     |
| 1:A:92:PHE:CB   | 1:A:100:ILE:CD1  | 0.46     | 2.94        | 14     | 15    |
| 1:A:469:SER:O   | 1:A:472:PHE:N    | 0.46     | 2.49        | 2      | 3     |
| 1:A:22:ASP:OD1  | 1:A:24:ASN:CB    | 0.46     | 2.64        | 4      | 4     |
| 1:A:51:LEU:HD21 | 1:A:471:MET:SD   | 0.46     | 2.51        | 4      | 2     |
| 1:A:114:GLU:O   | 1:A:115:LYS:CG   | 0.46     | 2.64        | 5      | 2     |
| 1:A:114:GLU:C   | 1:A:115:LYS:CG   | 0.46     | 2.89        | 12     | 2     |
| 1:A:464:ALA:O   | 1:A:468:VAL:CG2  | 0.46     | 2.59        | 5      | 3     |
| 1:A:90:LYS:CB   | 1:A:90:LYS:NZ    | 0.46     | 2.79        | 19     | 1     |
| 1:A:117:THR:C   | 1:A:119:ALA:N    | 0.45     | 2.74        | 9      | 7     |
| 1:A:89:PHE:CE2  | 1:A:137:ILE:HB   | 0.45     | 2.46        | 12     | 3     |
| 1:A:50:ASP:OD1  | 1:A:50:ASP:C     | 0.45     | 2.59        | 3      | 1     |
| 1:A:103:ALA:O   | 1:A:107:HIS:HB3  | 0.45     | 2.11        | 19     | 7     |
| 1:A:22:ASP:OD1  | 1:A:24:ASN:N     | 0.45     | 2.50        | 3      | 17    |
| 1:A:35:VAL:O    | 1:A:38:SER:N     | 0.45     | 2.49        | 1      | 14    |
| 1:A:47:GLU:O    | 1:A:48:VAL:C     | 0.45     | 2.59        | 12     | 20    |
| 1:A:134:GLU:O   | 1:A:139:GLN:NE2  | 0.45     | 2.50        | 11     | 8     |
| 1:A:71:LEU:O    | 1:A:74:ARG:N     | 0.45     | 2.49        | 18     | 3     |
| 1:A:24:ASN:OD1  | 1:A:25:GLY:N     | 0.45     | 2.50        | 6      | 3     |
| 1:A:136:ASN:OD1 | 1:A:139:GLN:CD   | 0.45     | 2.59        | 10     | 1     |
| 1:A:105:LEU:CD1 | 1:A:109:LEU:HD23 | 0.45     | 2.41        | 12     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:456:LYS:NZ  | 1:A:460:ASN:HD22 | 0.45     | 2.09        | 20     | 1     |
| 1:A:128:VAL:HB  | 1:A:142:ALA:HB3  | 0.45     | 1.86        | 1      | 1     |
| 1:A:108:VAL:O   | 1:A:111:SER:N    | 0.45     | 2.50        | 3      | 2     |
| 1:A:72:MET:CE   | 1:A:467:LYS:CD   | 0.45     | 2.94        | 5      | 2     |
| 1:A:28:SER:OG   | 1:A:61:HIS:NE2   | 0.45     | 2.49        | 12     | 1     |
| 1:A:55:ILE:CD1  | 1:A:471:MET:SD   | 0.45     | 3.04        | 19     | 2     |
| 1:A:131:GLY:O   | 1:A:132:SER:C    | 0.45     | 2.60        | 18     | 1     |
| 1:A:17:ALA:O    | 1:A:18:LEU:C     | 0.45     | 2.59        | 11     | 5     |
| 1:A:25:GLY:O    | 1:A:64:GLU:CG    | 0.45     | 2.65        | 13     | 9     |
| 1:A:35:VAL:O    | 1:A:36:MET:C     | 0.45     | 2.59        | 11     | 12    |
| 1:A:117:THR:O   | 1:A:120:GLU:N    | 0.45     | 2.50        | 5      | 9     |
| 1:A:475:LEU:O   | 1:A:476:ARG:C    | 0.45     | 2.60        | 14     | 8     |
| 1:A:5:THR:O     | 1:A:8:GLN:N      | 0.45     | 2.50        | 10     | 10    |
| 1:A:11:GLU:CD   | 1:A:456:LYS:HZ1  | 0.45     | 2.20        | 8      | 1     |
| 1:A:136:ASN:O   | 1:A:137:ILE:C    | 0.45     | 2.58        | 13     | 1     |
| 1:A:8:GLN:CD    | 1:A:11:GLU:OE2   | 0.45     | 2.60        | 15     | 1     |
| 1:A:50:ASP:O    | 1:A:54:GLU:CD    | 0.45     | 2.60        | 1      | 1     |
| 1:A:119:ALA:O   | 1:A:123:ASP:N    | 0.45     | 2.50        | 10     | 1     |
| 1:A:44:SER:O    | 1:A:47:GLU:N     | 0.45     | 2.50        | 20     | 1     |
| 1:A:11:GLU:C    | 1:A:13:LYS:N     | 0.45     | 2.74        | 18     | 10    |
| 1:A:43:PRO:HB3  | 1:A:472:PHE:CD1  | 0.45     | 2.46        | 6      | 1     |
| 1:A:106:LYS:CD  | 1:A:121:VAL:HG11 | 0.45     | 2.41        | 6      | 1     |
| 1:A:13:LYS:CE   | 1:A:65:PHE:CE2   | 0.45     | 3.00        | 10     | 1     |
| 1:A:51:LEU:CD1  | 1:A:471:MET:SD   | 0.45     | 3.05        | 10     | 1     |
| 1:A:49:ASN:OD1  | 1:A:61:HIS:ND1   | 0.45     | 2.50        | 12     | 1     |
| 1:A:106:LYS:O   | 1:A:107:HIS:C    | 0.45     | 2.60        | 14     | 8     |
| 1:A:29:SER:HB3  | 1:A:61:HIS:CE1   | 0.45     | 2.46        | 8      | 1     |
| 1:A:129:SER:OG  | 1:A:133:GLY:N    | 0.45     | 2.50        | 12     | 1     |
| 1:A:112:ILE:CD1 | 1:A:461:LYS:HG2  | 0.45     | 2.42        | 8      | 12    |
| 1:A:143:LEU:C   | 1:A:145:SER:N    | 0.45     | 2.73        | 11     | 3     |
| 1:A:464:ALA:O   | 1:A:468:VAL:N    | 0.45     | 2.49        | 14     | 7     |
| 1:A:85:LEU:HD11 | 1:A:141:ALA:HA   | 0.45     | 1.89        | 11     | 1     |
| 1:A:28:SER:OG   | 1:A:61:HIS:CD2   | 0.45     | 2.70        | 12     | 1     |
| 1:A:129:SER:OG  | 1:A:132:SER:N    | 0.45     | 2.50        | 12     | 1     |
| 1:A:460:ASN:O   | 1:A:463:LEU:N    | 0.45     | 2.50        | 15     | 1     |
| 1:A:33:ALA:O    | 1:A:37:ARG:NE    | 0.45     | 2.50        | 18     | 1     |
| 1:A:102:ALA:O   | 1:A:106:LYS:N    | 0.45     | 2.50        | 11     | 6     |
| 1:A:28:SER:OG   | 1:A:29:SER:N     | 0.45     | 2.49        | 12     | 1     |
| 1:A:9:ILE:C     | 1:A:11:GLU:N     | 0.45     | 2.72        | 16     | 1     |
| 1:A:72:MET:CA   | 1:A:467:LYS:NZ   | 0.45     | 2.80        | 17     | 1     |
| 1:A:51:LEU:HD21 | 1:A:471:MET:CB   | 0.45     | 2.41        | 5      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:119:ALA:O    | 1:A:123:ASP:CB   | 0.45     | 2.64        | 11     | 2     |
| 1:A:112:ILE:CD1  | 1:A:461:LYS:HG3  | 0.45     | 2.42        | 12     | 1     |
| 1:A:459:ARG:C    | 1:A:463:LEU:HD13 | 0.45     | 2.37        | 12     | 1     |
| 1:A:19:PHE:CD2   | 1:A:27:ILE:HD13  | 0.45     | 2.46        | 14     | 1     |
| 1:A:470:ARG:O    | 1:A:471:MET:C    | 0.45     | 2.59        | 15     | 2     |
| 1:A:19:PHE:CE1   | 1:A:35:VAL:CG1   | 0.45     | 3.00        | 20     | 1     |
| 1:A:462:ILE:O    | 1:A:463:LEU:C    | 0.44     | 2.60        | 19     | 5     |
| 1:A:74:ARG:O     | 1:A:74:ARG:CD    | 0.44     | 2.66        | 15     | 2     |
| 1:A:116:LEU:HD13 | 1:A:124:MET:HE1  | 0.44     | 1.89        | 8      | 2     |
| 1:A:60:ASN:O     | 1:A:61:HIS:C     | 0.44     | 2.60        | 19     | 1     |
| 1:A:22:ASP:OD1   | 1:A:22:ASP:C     | 0.44     | 2.59        | 1      | 2     |
| 1:A:35:VAL:HG12  | 1:A:36:MET:N     | 0.44     | 2.26        | 19     | 2     |
| 1:A:102:ALA:O    | 1:A:106:LYS:CG   | 0.44     | 2.66        | 9      | 4     |
| 1:A:58:ASP:OD2   | 1:A:60:ASN:CG    | 0.44     | 2.60        | 9      | 4     |
| 1:A:102:ALA:O    | 1:A:103:ALA:C    | 0.44     | 2.60        | 13     | 19    |
| 1:A:455:ARG:O    | 1:A:458:LEU:N    | 0.44     | 2.50        | 1      | 2     |
| 1:A:47:GLU:O     | 1:A:49:ASN:N     | 0.44     | 2.51        | 12     | 6     |
| 1:A:470:ARG:HD2  | 1:A:474:VAL:CG2  | 0.44     | 2.43        | 15     | 1     |
| 1:A:475:LEU:C    | 1:A:475:LEU:HD12 | 0.44     | 2.37        | 3      | 1     |
| 1:A:71:LEU:C     | 1:A:73:SER:N     | 0.44     | 2.75        | 10     | 1     |
| 1:A:465:ILE:O    | 1:A:469:SER:CB   | 0.44     | 2.65        | 4      | 4     |
| 1:A:113:GLY:O    | 1:A:115:LYS:CG   | 0.44     | 2.65        | 3      | 1     |
| 1:A:463:LEU:HB3  | 1:A:467:LYS:HZ2  | 0.44     | 1.72        | 10     | 1     |
| 1:A:117:THR:OG1  | 1:A:120:GLU:CD   | 0.44     | 2.60        | 15     | 1     |
| 1:A:85:LEU:O     | 1:A:86:LEU:C     | 0.44     | 2.60        | 4      | 1     |
| 1:A:470:ARG:C    | 1:A:472:PHE:N    | 0.44     | 2.74        | 17     | 5     |
| 1:A:47:GLU:O     | 1:A:51:LEU:N     | 0.44     | 2.50        | 16     | 5     |
| 1:A:44:SER:C     | 1:A:46:ALA:N     | 0.44     | 2.74        | 20     | 3     |
| 1:A:116:LEU:HD22 | 1:A:124:MET:HE2  | 0.44     | 1.90        | 11     | 1     |
| 1:A:114:GLU:OE2  | 1:A:116:LEU:CG   | 0.44     | 2.66        | 12     | 1     |
| 1:A:136:ASN:O    | 1:A:138:GLN:N    | 0.44     | 2.51        | 13     | 1     |
| 1:A:457:ALA:O    | 1:A:461:LYS:NZ   | 0.44     | 2.49        | 19     | 1     |
| 1:A:123:ASP:OD1  | 1:A:123:ASP:C    | 0.44     | 2.60        | 5      | 1     |
| 1:A:19:PHE:CD2   | 1:A:35:VAL:CG2   | 0.44     | 3.00        | 12     | 1     |
| 1:A:462:ILE:HA   | 1:A:465:ILE:HD12 | 0.44     | 1.90        | 15     | 1     |
| 1:A:7:GLU:OE2    | 1:A:456:LYS:NZ   | 0.44     | 2.51        | 16     | 1     |
| 1:A:466:ALA:O    | 1:A:470:ARG:N    | 0.43     | 2.50        | 1      | 2     |
| 1:A:11:GLU:CD    | 1:A:456:LYS:NZ   | 0.43     | 2.76        | 7      | 2     |
| 1:A:66:SER:O     | 1:A:70:ALA:HB2   | 0.43     | 2.13        | 10     | 1     |
| 1:A:15:ALA:HB2   | 1:A:460:ASN:OD1  | 0.43     | 2.13        | 14     | 1     |
| 1:A:56:ASP:OD2   | 1:A:59:GLY:CA    | 0.43     | 2.66        | 20     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:116:LEU:CD2  | 1:A:124:MET:HE2  | 0.43     | 2.42        | 19     | 1     |
| 1:A:20:ASP:O     | 1:A:23:ASN:ND2   | 0.43     | 2.51        | 1      | 4     |
| 1:A:92:PHE:HB3   | 1:A:100:ILE:HD13 | 0.43     | 1.89        | 14     | 7     |
| 1:A:56:ASP:CG    | 1:A:62:GLN:O     | 0.43     | 2.61        | 12     | 2     |
| 1:A:16:PHE:CE1   | 1:A:64:GLU:O     | 0.43     | 2.72        | 7      | 2     |
| 1:A:105:LEU:HD13 | 1:A:125:LEU:HD11 | 0.43     | 1.90        | 17     | 1     |
| 1:A:124:MET:HE1  | 1:A:458:LEU:HD11 | 0.43     | 1.90        | 12     | 1     |
| 1:A:112:ILE:HD13 | 1:A:461:LYS:HG2  | 0.43     | 1.89        | 1      | 1     |
| 1:A:15:ALA:HA    | 1:A:18:LEU:CD1   | 0.43     | 2.43        | 2      | 11    |
| 1:A:22:ASP:OD1   | 1:A:24:ASN:CG    | 0.43     | 2.61        | 3      | 3     |
| 1:A:128:VAL:HG21 | 1:A:139:GLN:O    | 0.43     | 2.14        | 10     | 2     |
| 1:A:87:GLU:HB2   | 1:A:466:ALA:HB1  | 0.43     | 1.89        | 15     | 1     |
| 1:A:95:ASN:OD1   | 1:A:95:ASN:C     | 0.43     | 2.59        | 20     | 2     |
| 1:A:11:GLU:OE2   | 1:A:456:LYS:NZ   | 0.43     | 2.51        | 7      | 1     |
| 1:A:464:ALA:O    | 1:A:468:VAL:HG13 | 0.43     | 2.14        | 11     | 2     |
| 1:A:55:ILE:N     | 1:A:55:ILE:CD1   | 0.43     | 2.69        | 10     | 1     |
| 1:A:474:VAL:HG13 | 1:A:475:LEU:N    | 0.43     | 2.29        | 9      | 5     |
| 1:A:72:MET:N     | 1:A:72:MET:SD    | 0.43     | 2.91        | 11     | 3     |
| 1:A:11:GLU:OE1   | 1:A:456:LYS:CD   | 0.43     | 2.67        | 18     | 1     |
| 1:A:8:GLN:OE1    | 1:A:11:GLU:CD    | 0.43     | 2.61        | 5      | 1     |
| 1:A:466:ALA:O    | 1:A:469:SER:CB   | 0.43     | 2.67        | 7      | 2     |
| 1:A:471:MET:HA   | 1:A:474:VAL:HG12 | 0.43     | 1.90        | 13     | 5     |
| 1:A:36:MET:HE2   | 1:A:41:LEU:HD13  | 0.43     | 1.90        | 15     | 1     |
| 1:A:469:SER:O    | 1:A:471:MET:N    | 0.43     | 2.51        | 20     | 1     |
| 1:A:105:LEU:HD23 | 1:A:121:VAL:HG22 | 0.43     | 1.86        | 6      | 1     |
| 1:A:109:LEU:CD1  | 1:A:458:LEU:HD11 | 0.43     | 2.44        | 13     | 1     |
| 1:A:33:ALA:CB    | 1:A:37:ARG:HH21  | 0.43     | 2.26        | 18     | 1     |
| 1:A:464:ALA:O    | 1:A:466:ALA:N    | 0.43     | 2.52        | 4      | 3     |
| 1:A:32:LEU:HD11  | 1:A:51:LEU:CD1   | 0.43     | 2.43        | 13     | 1     |
| 1:A:22:ASP:C     | 1:A:23:ASN:CG    | 0.43     | 2.87        | 15     | 1     |
| 1:A:57:VAL:HG23  | 1:A:67:GLU:HG2   | 0.42     | 1.91        | 4      | 2     |
| 1:A:97:ASP:OD1   | 1:A:99:LEU:O     | 0.42     | 2.36        | 4      | 2     |
| 1:A:102:ALA:HB2  | 1:A:125:LEU:HD11 | 0.42     | 1.90        | 14     | 1     |
| 1:A:474:VAL:O    | 1:A:476:ARG:N    | 0.42     | 2.52        | 2      | 2     |
| 1:A:21:LYS:NZ    | 1:A:34:THR:HG21  | 0.42     | 2.29        | 8      | 1     |
| 1:A:116:LEU:HD22 | 1:A:124:MET:CE   | 0.42     | 2.44        | 14     | 1     |
| 1:A:114:GLU:CD   | 1:A:116:LEU:HD13 | 0.42     | 2.38        | 17     | 1     |
| 1:A:462:ILE:O    | 1:A:466:ALA:N    | 0.42     | 2.51        | 19     | 1     |
| 1:A:92:PHE:HE2   | 1:A:105:LEU:HD13 | 0.42     | 1.74        | 1      | 1     |
| 1:A:114:GLU:HG3  | 1:A:461:LYS:HZ3  | 0.42     | 1.74        | 8      | 1     |
| 1:A:125:LEU:HD13 | 1:A:125:LEU:N    | 0.42     | 2.29        | 17     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:470:ARG:C    | 1:A:470:ARG:CD   | 0.42     | 2.92        | 6      | 1     |
| 1:A:85:LEU:HD11  | 1:A:141:ALA:N    | 0.42     | 2.29        | 10     | 1     |
| 1:A:460:ASN:C    | 1:A:462:ILE:N    | 0.42     | 2.73        | 15     | 1     |
| 1:A:470:ARG:HD3  | 1:A:474:VAL:CG2  | 0.42     | 2.44        | 15     | 3     |
| 1:A:470:ARG:HD3  | 1:A:474:VAL:HG23 | 0.42     | 1.91        | 20     | 1     |
| 1:A:5:THR:O      | 1:A:6:GLU:C      | 0.42     | 2.61        | 18     | 7     |
| 1:A:129:SER:O    | 1:A:132:SER:CB   | 0.42     | 2.67        | 4      | 3     |
| 1:A:13:LYS:HE3   | 1:A:65:PHE:CE2   | 0.42     | 2.50        | 10     | 1     |
| 1:A:462:ILE:C    | 1:A:464:ALA:N    | 0.42     | 2.77        | 15     | 1     |
| 1:A:12:PHE:O     | 1:A:13:LYS:C     | 0.42     | 2.62        | 16     | 1     |
| 1:A:85:LEU:O     | 1:A:88:ALA:N     | 0.42     | 2.53        | 4      | 1     |
| 1:A:49:ASN:OD1   | 1:A:61:HIS:NE2   | 0.42     | 2.50        | 10     | 1     |
| 1:A:460:ASN:O    | 1:A:460:ASN:OD1  | 0.42     | 2.38        | 10     | 1     |
| 1:A:92:PHE:HB3   | 1:A:100:ILE:CD1  | 0.42     | 2.44        | 14     | 1     |
| 1:A:471:MET:C    | 1:A:474:VAL:HG12 | 0.42     | 2.38        | 14     | 1     |
| 1:A:85:LEU:O     | 1:A:89:PHE:CB    | 0.42     | 2.68        | 16     | 1     |
| 1:A:102:ALA:O    | 1:A:106:LYS:HG3  | 0.42     | 2.15        | 9      | 6     |
| 1:A:120:GLU:OE2  | 1:A:120:GLU:CA   | 0.42     | 2.67        | 2      | 1     |
| 1:A:136:ASN:OD1  | 1:A:139:GLN:OE1  | 0.42     | 2.38        | 10     | 3     |
| 1:A:85:LEU:HG    | 1:A:141:ALA:CB   | 0.42     | 2.45        | 1      | 2     |
| 1:A:56:ASP:OD1   | 1:A:60:ASN:OD1   | 0.42     | 2.38        | 2      | 10    |
| 1:A:11:GLU:OE1   | 1:A:456:LYS:CE   | 0.42     | 2.68        | 4      | 1     |
| 1:A:60:ASN:OD1   | 1:A:60:ASN:C     | 0.42     | 2.62        | 20     | 1     |
| 1:A:72:MET:O     | 1:A:467:LYS:NZ   | 0.42     | 2.52        | 4      | 1     |
| 1:A:98:GLY:C     | 1:A:99:LEU:HG    | 0.42     | 2.39        | 14     | 4     |
| 1:A:5:THR:C      | 1:A:7:GLU:N      | 0.42     | 2.75        | 16     | 2     |
| 1:A:109:LEU:HD12 | 1:A:114:GLU:CG   | 0.42     | 2.45        | 16     | 1     |
| 1:A:105:LEU:CD2  | 1:A:124:MET:SD   | 0.42     | 3.08        | 17     | 1     |
| 1:A:39:LEU:HD11  | 1:A:465:ILE:HG23 | 0.42     | 1.87        | 18     | 1     |
| 1:A:71:LEU:O     | 1:A:72:MET:C     | 0.42     | 2.63        | 18     | 1     |
| 1:A:456:LYS:CD   | 1:A:456:LYS:C    | 0.42     | 2.92        | 20     | 1     |
| 1:A:97:ASP:O     | 1:A:97:ASP:CG    | 0.42     | 2.63        | 18     | 3     |
| 1:A:112:ILE:HG21 | 1:A:465:ILE:CG1  | 0.42     | 2.45        | 4      | 1     |
| 1:A:125:LEU:C    | 1:A:129:SER:HB3  | 0.42     | 2.40        | 18     | 1     |
| 1:A:129:SER:O    | 1:A:132:SER:OG   | 0.41     | 2.39        | 8      | 1     |
| 1:A:128:VAL:CG1  | 1:A:142:ALA:CB   | 0.41     | 2.98        | 10     | 1     |
| 1:A:463:LEU:CB   | 1:A:467:LYS:HZ2  | 0.41     | 2.28        | 10     | 1     |
| 1:A:15:ALA:C     | 1:A:68:PHE:CE2   | 0.41     | 2.98        | 13     | 1     |
| 1:A:39:LEU:HD23  | 1:A:111:SER:HG   | 0.41     | 1.75        | 1      | 1     |
| 1:A:66:SER:O     | 1:A:69:LEU:HD12  | 0.41     | 2.15        | 13     | 2     |
| 1:A:19:PHE:CE1   | 1:A:35:VAL:HG11  | 0.41     | 2.49        | 20     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:14:GLU:C     | 1:A:16:PHE:N     | 0.41     | 2.77        | 5      | 3     |
| 1:A:95:ASN:ND2   | 1:A:95:ASN:O     | 0.41     | 2.53        | 13     | 4     |
| 1:A:461:LYS:HE2  | 1:A:461:LYS:CA   | 0.41     | 2.45        | 4      | 1     |
| 1:A:106:LYS:HG2  | 1:A:121:VAL:HG11 | 0.41     | 1.92        | 5      | 1     |
| 1:A:112:ILE:HD12 | 1:A:461:LYS:HD3  | 0.41     | 1.92        | 6      | 1     |
| 1:A:125:LEU:N    | 1:A:125:LEU:HD13 | 0.41     | 2.30        | 8      | 1     |
| 1:A:112:ILE:CD1  | 1:A:461:LYS:HD3  | 0.41     | 2.44        | 10     | 1     |
| 1:A:144:LEU:N    | 1:A:144:LEU:HD23 | 0.41     | 2.30        | 13     | 1     |
| 1:A:58:ASP:OD2   | 1:A:67:GLU:OE2   | 0.41     | 2.38        | 8      | 1     |
| 1:A:105:LEU:HD13 | 1:A:125:LEU:CD2  | 0.41     | 2.46        | 9      | 1     |
| 1:A:104:GLU:O    | 1:A:108:VAL:CG2  | 0.41     | 2.68        | 11     | 1     |
| 1:A:36:MET:CE    | 1:A:472:PHE:HB2  | 0.41     | 2.46        | 1      | 2     |
| 1:A:101:SER:O    | 1:A:102:ALA:C    | 0.41     | 2.63        | 14     | 2     |
| 1:A:19:PHE:O     | 1:A:21:LYS:CD    | 0.41     | 2.68        | 20     | 2     |
| 1:A:14:GLU:O     | 1:A:17:ALA:N     | 0.41     | 2.54        | 8      | 1     |
| 1:A:103:ALA:HA   | 1:A:106:LYS:CG   | 0.41     | 2.46        | 18     | 1     |
| 1:A:475:LEU:C    | 1:A:475:LEU:CD1  | 0.41     | 2.90        | 20     | 1     |
| 1:A:55:ILE:CG2   | 1:A:71:LEU:HD13  | 0.41     | 2.44        | 2      | 1     |
| 1:A:13:LYS:HE2   | 1:A:65:PHE:CD2   | 0.41     | 2.50        | 5      | 1     |
| 1:A:55:ILE:CG2   | 1:A:71:LEU:HD12  | 0.41     | 2.45        | 7      | 1     |
| 1:A:88:ALA:O     | 1:A:91:VAL:HG12  | 0.41     | 2.16        | 10     | 1     |
| 1:A:128:VAL:HG21 | 1:A:142:ALA:HB3  | 0.41     | 1.93        | 10     | 1     |
| 1:A:71:LEU:CD2   | 1:A:471:MET:CE   | 0.41     | 2.98        | 16     | 1     |
| 1:A:87:GLU:HA    | 1:A:90:LYS:HZ2   | 0.41     | 1.76        | 2      | 1     |
| 1:A:12:PHE:CG    | 1:A:69:LEU:HB2   | 0.41     | 2.50        | 18     | 3     |
| 1:A:456:LYS:CB   | 1:A:456:LYS:NZ   | 0.41     | 2.84        | 4      | 1     |
| 1:A:117:THR:O    | 1:A:118:ASP:C    | 0.41     | 2.63        | 10     | 1     |
| 1:A:124:MET:O    | 1:A:143:LEU:HD21 | 0.41     | 2.16        | 10     | 1     |
| 1:A:118:ASP:OD2  | 1:A:118:ASP:C    | 0.41     | 2.63        | 15     | 1     |
| 1:A:38:SER:O     | 1:A:111:SER:OG   | 0.41     | 2.39        | 18     | 2     |
| 1:A:135:ILE:HG22 | 1:A:139:GLN:HE21 | 0.41     | 1.75        | 5      | 1     |
| 1:A:11:GLU:O     | 1:A:12:PHE:C     | 0.41     | 2.64        | 9      | 1     |
| 1:A:128:VAL:CG1  | 1:A:142:ALA:HB1  | 0.41     | 2.46        | 10     | 1     |
| 1:A:29:SER:CB    | 1:A:61:HIS:CE1   | 0.41     | 3.03        | 12     | 1     |
| 1:A:50:ASP:O     | 1:A:54:GLU:CG    | 0.41     | 2.69        | 1      | 1     |
| 1:A:72:MET:HA    | 1:A:467:LYS:CE   | 0.41     | 2.46        | 1      | 1     |
| 1:A:87:GLU:CD    | 1:A:90:LYS:NZ    | 0.41     | 2.79        | 2      | 1     |
| 1:A:61:HIS:C     | 1:A:62:GLN:HG3   | 0.41     | 2.40        | 6      | 1     |
| 1:A:128:VAL:HG22 | 1:A:143:LEU:HD21 | 0.40     | 1.93        | 11     | 1     |
| 1:A:91:VAL:O     | 1:A:94:LYS:NZ    | 0.40     | 2.51        | 14     | 1     |
| 1:A:33:ALA:O     | 1:A:37:ARG:CG    | 0.40     | 2.69        | 20     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:139:GLN:O   | 1:A:140:PHE:C    | 0.40     | 2.65        | 2      | 2     |
| 1:A:106:LYS:O   | 1:A:110:THR:N    | 0.40     | 2.55        | 2      | 1     |
| 1:A:456:LYS:NZ  | 1:A:456:LYS:CB   | 0.40     | 2.84        | 3      | 1     |
| 1:A:65:PHE:O    | 1:A:69:LEU:HD23  | 0.40     | 2.16        | 18     | 1     |
| 1:A:26:SER:CB   | 1:A:62:GLN:OE1   | 0.40     | 2.69        | 6      | 1     |
| 1:A:57:VAL:HG12 | 1:A:67:GLU:CD    | 0.40     | 2.42        | 11     | 1     |
| 1:A:36:MET:HE1  | 1:A:472:PHE:CD2  | 0.40     | 2.51        | 17     | 1     |
| 1:A:114:GLU:OE2 | 1:A:116:LEU:HD13 | 0.40     | 2.16        | 17     | 1     |
| 1:A:32:LEU:HD23 | 1:A:32:LEU:C     | 0.40     | 2.41        | 2      | 1     |
| 1:A:126:ARG:O   | 1:A:127:GLU:C    | 0.40     | 2.64        | 8      | 1     |
| 1:A:107:HIS:O   | 1:A:111:SER:OG   | 0.40     | 2.39        | 14     | 1     |
| 1:A:72:MET:CB   | 1:A:467:LYS:NZ   | 0.40     | 2.83        | 17     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed        | Favoured      | Allowed      | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|--------------|------------|-------------|----|
| 1   | A     | 152/176 (86%)   | 118±2 (77±1%) | 31±2 (21±1%) | 3±1 (2±1%) | 8           | 48 |
| All | All   | 3040/3520 (86%) | 2350 (77%)    | 626 (21%)    | 64 (2%)    | 8           | 48 |

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 104 | GLU  | 19             |
| 1   | A     | 126 | ARG  | 19             |
| 1   | A     | 20  | ASP  | 17             |
| 1   | A     | 114 | GLU  | 3              |
| 1   | A     | 468 | VAL  | 3              |
| 1   | A     | 132 | SER  | 2              |
| 1   | A     | 470 | ARG  | 1              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric    | Outliers     | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|-------------|----|
| 1   | A     | 130/150 (87%)   | 97±3 (75±2%) | 33±3 (25±2%) | 2           | 25 |
| All | All   | 2600/3000 (87%) | 1949 (75%)   | 651 (25%)    | 2           | 25 |

All 71 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     | 34  | THR  | 20             |
| 1   | A     | 63  | ILE  | 20             |
| 1   | A     | 69  | LEU  | 20             |
| 1   | A     | 93  | ASP  | 20             |
| 1   | A     | 95  | ASN  | 20             |
| 1   | A     | 97  | ASP  | 20             |
| 1   | A     | 107 | HIS  | 20             |
| 1   | A     | 108 | VAL  | 20             |
| 1   | A     | 136 | ASN  | 20             |
| 1   | A     | 475 | LEU  | 20             |
| 1   | A     | 35  | VAL  | 19             |
| 1   | A     | 111 | SER  | 19             |
| 1   | A     | 458 | LEU  | 19             |
| 1   | A     | 9   | ILE  | 18             |
| 1   | A     | 94  | LYS  | 18             |
| 1   | A     | 106 | LYS  | 18             |
| 1   | A     | 51  | LEU  | 18             |
| 1   | A     | 26  | SER  | 16             |
| 1   | A     | 32  | LEU  | 16             |
| 1   | A     | 72  | MET  | 16             |
| 1   | A     | 85  | LEU  | 15             |
| 1   | A     | 461 | LYS  | 15             |
| 1   | A     | 30  | SER  | 14             |
| 1   | A     | 456 | LYS  | 14             |
| 1   | A     | 91  | VAL  | 14             |
| 1   | A     | 20  | ASP  | 13             |
| 1   | A     | 64  | GLU  | 12             |
| 1   | A     | 47  | GLU  | 12             |
| 1   | A     | 105 | LEU  | 11             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 144 | LEU  | 11             |
| 1   | A     | 476 | ARG  | 10             |
| 1   | A     | 99  | LEU  | 9              |
| 1   | A     | 55  | ILE  | 8              |
| 1   | A     | 123 | ASP  | 7              |
| 1   | A     | 44  | SER  | 6              |
| 1   | A     | 50  | ASP  | 6              |
| 1   | A     | 109 | LEU  | 6              |
| 1   | A     | 121 | VAL  | 6              |
| 1   | A     | 143 | LEU  | 5              |
| 1   | A     | 463 | LEU  | 5              |
| 1   | A     | 13  | LYS  | 5              |
| 1   | A     | 469 | SER  | 5              |
| 1   | A     | 118 | ASP  | 5              |
| 1   | A     | 470 | ARG  | 5              |
| 1   | A     | 115 | LYS  | 5              |
| 1   | A     | 471 | MET  | 4              |
| 1   | A     | 29  | SER  | 4              |
| 1   | A     | 114 | GLU  | 4              |
| 1   | A     | 116 | LEU  | 4              |
| 1   | A     | 53  | ASN  | 3              |
| 1   | A     | 145 | SER  | 3              |
| 1   | A     | 125 | LEU  | 3              |
| 1   | A     | 90  | LYS  | 3              |
| 1   | A     | 42  | SER  | 2              |
| 1   | A     | 74  | ARG  | 2              |
| 1   | A     | 86  | LEU  | 2              |
| 1   | A     | 467 | LYS  | 2              |
| 1   | A     | 38  | SER  | 1              |
| 1   | A     | 120 | GLU  | 1              |
| 1   | A     | 71  | LEU  | 1              |
| 1   | A     | 28  | SER  | 1              |
| 1   | A     | 58  | ASP  | 1              |
| 1   | A     | 54  | GLU  | 1              |
| 1   | A     | 73  | SER  | 1              |
| 1   | A     | 101 | SER  | 1              |
| 1   | A     | 129 | SER  | 1              |
| 1   | A     | 124 | MET  | 1              |
| 1   | A     | 8   | GLN  | 1              |
| 1   | A     | 135 | ILE  | 1              |
| 1   | A     | 459 | ARG  | 1              |
| 1   | A     | 49  | ASN  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 94% 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                  | 2204 |
| Number of shifts mapped to atoms        | 2204 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 3    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 176      | $-0.42 \pm 0.10$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 165      | $0.18 \pm 0.06$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 165      | $-0.48 \pm 0.11$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 175      | $0.32 \pm 0.29$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 1944 atoms were assigned a chemical shift out of a possible 2061. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 764/771 (99%)   | 313/313 (100%) | 299/306 (98%)   | 152/152 (100%)  |
| Sidechain | 1103/1186 (93%) | 741/771 (96%)  | 343/373 (92%)   | 19/42 (45%)     |

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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 | 77/104 (74%)    | 48/53 (91%)          | 29/49 (59%)           | 0/2 (0%)              |
| Overall  | 1944/2061 (94%) | 1102/1137 (97%)      | 671/728 (92%)         | 171/196 (87%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 94%, i.e. 2197 atoms were assigned a chemical shift out of a possible 2331. 0 out of 30 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  | 877/889 (99%)   | 361/362 (100%)       | 341/352 (97%)         | 175/175 (100%)        |
| Sidechain | 1243/1338 (93%) | 832/866 (96%)        | 387/421 (92%)         | 24/51 (47%)           |
| Aromatic  | 77/104 (74%)    | 48/53 (91%)          | 29/49 (59%)           | 0/2 (0%)              |
| Overall   | 2197/2331 (94%) | 1241/1281 (97%)      | 757/822 (92%)         | 199/228 (87%)         |

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

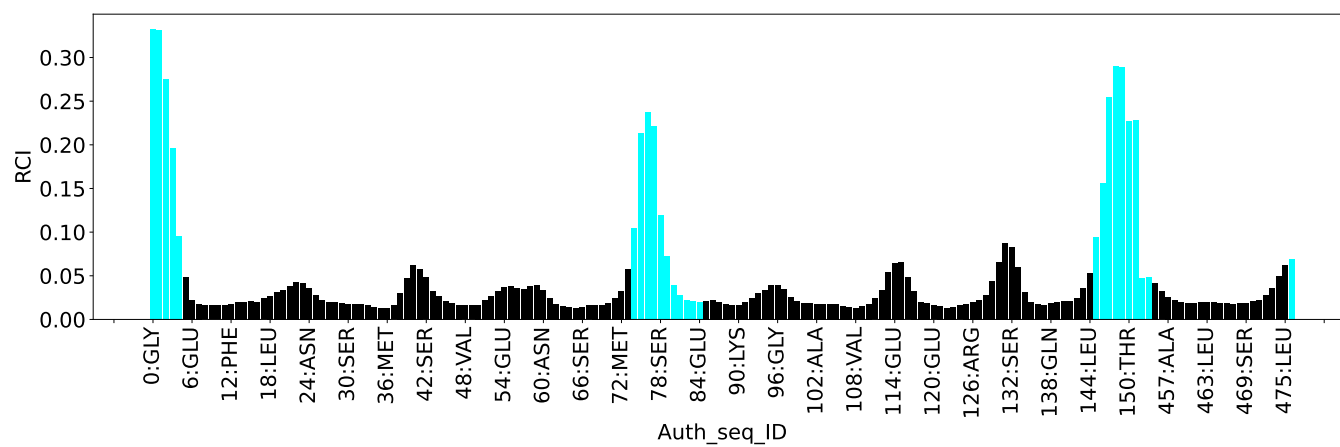
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 5   | THR  | HG1  | 5.66       | 0.08 – 2.19         | 21.4    |
| 1       | A     | 34  | THR  | HG1  | 5.56       | 0.08 – 2.19         | 21.0    |
| 1       | A     | 110 | THR  | HG1  | 5.18       | 0.08 – 2.19         | 19.1    |

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 3899  |
| Intra-residue ( $ i-j =0$ )                              | 1008  |
| Sequential ( $ i-j =1$ )                                 | 989   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 997   |
| Long range ( $ i-j \geq 5$ )                             | 905   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 267   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 23.3  |
| Number of long range restraints per residue <sup>1</sup> | 5.1   |

<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)  | 10.0                                   | 0.2     |
| 0.2-0.5 (Medium) | 3.3                                    | 0.49    |
| >0.5 (Large)     | 1.1                                    | 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)   | 6.2                                    | 5.13    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis

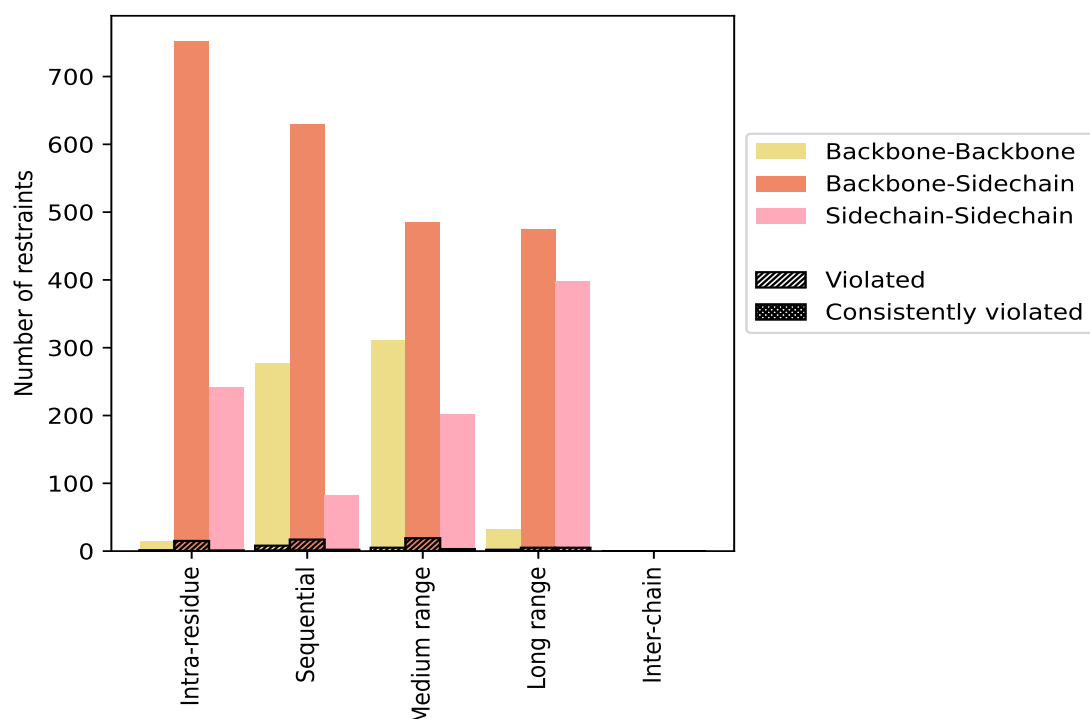
### 9.1 Summary of distance violations

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>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">1008</a> | <a href="#">25.9</a>  | <a href="#">17</a>    | <a href="#">1.7</a> | <a href="#">0.4</a> | <a href="#">1</a>                  | <a href="#">0.1</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 14                   | 0.4                   | 1                     | 7.1                 | 0.0                 | 1                                  | 7.1                 | 0.0                 |
| Backbone-Sidechain                                         | 752                  | 19.3                  | 15                    | 2.0                 | 0.4                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 242                  | 6.2                   | 1                     | 0.4                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">989</a>  | <a href="#">25.4</a>  | <a href="#">27</a>    | <a href="#">2.7</a> | <a href="#">0.7</a> | <a href="#">2</a>                  | <a href="#">0.2</a> | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 277                  | 7.1                   | 8                     | 2.9                 | 0.2                 | 1                                  | 0.4                 | 0.0                 |
| Backbone-Sidechain                                         | 630                  | 16.2                  | 17                    | 2.7                 | 0.4                 | 1                                  | 0.2                 | 0.0                 |
| Sidechain-Sidechain                                        | 82                   | 2.1                   | 2                     | 2.4                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">997</a>  | <a href="#">25.6</a>  | <a href="#">27</a>    | <a href="#">2.7</a> | <a href="#">0.7</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 311                  | 8.0                   | 5                     | 1.6                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 485                  | 12.4                  | 19                    | 3.9                 | 0.5                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 201                  | 5.2                   | 3                     | 1.5                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">905</a>  | <a href="#">23.2</a>  | <a href="#">12</a>    | <a href="#">1.3</a> | <a href="#">0.3</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 32                   | 0.8                   | 2                     | 6.2                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 475                  | 12.2                  | 5                     | 1.1                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 398                  | 10.2                  | 5                     | 1.3                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 0                    | 0.0                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 0                    | 0.0                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">3899</a> | <a href="#">100.0</a> | <a href="#">83</a>    | <a href="#">2.1</a> | <a href="#">2.1</a> | <a href="#">3</a>                  | <a href="#">0.1</a> | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 634                  | 16.3                  | 16                    | 2.5                 | 0.4                 | 2                                  | 0.3                 | 0.1                 |
| Backbone-Sidechain                                         | 2342                 | 60.1                  | 56                    | 2.4                 | 1.4                 | 1                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 923                  | 23.7                  | 11                    | 1.2                 | 0.3                 | 0                                  | 0.0                 | 0.0                 |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 4                    | 6               | 4               | 4               | 0               | 18    | 0.18     | 0.53    | 0.11                | 0.14       |
| 2        | 4                    | 8               | 3               | 0               | 0               | 15    | 0.2      | 0.62    | 0.13                | 0.14       |
| 3        | 4                    | 6               | 4               | 1               | 0               | 15    | 0.19     | 0.63    | 0.14                | 0.13       |
| 4        | 4                    | 4               | 4               | 2               | 0               | 14    | 0.21     | 0.57    | 0.13                | 0.16       |
| 5        | 3                    | 6               | 2               | 3               | 0               | 14    | 0.21     | 0.55    | 0.12                | 0.16       |
| 6        | 4                    | 5               | 3               | 0               | 0               | 12    | 0.23     | 0.49    | 0.13                | 0.18       |
| 7        | 5                    | 5               | 4               | 0               | 0               | 14    | 0.22     | 0.48    | 0.12                | 0.18       |
| 8        | 3                    | 3               | 5               | 2               | 0               | 13    | 0.22     | 0.58    | 0.16                | 0.12       |
| 9        | 3                    | 3               | 8               | 3               | 0               | 17    | 0.18     | 0.63    | 0.13                | 0.13       |
| 10       | 3                    | 8               | 8               | 1               | 0               | 20    | 0.17     | 0.57    | 0.11                | 0.13       |

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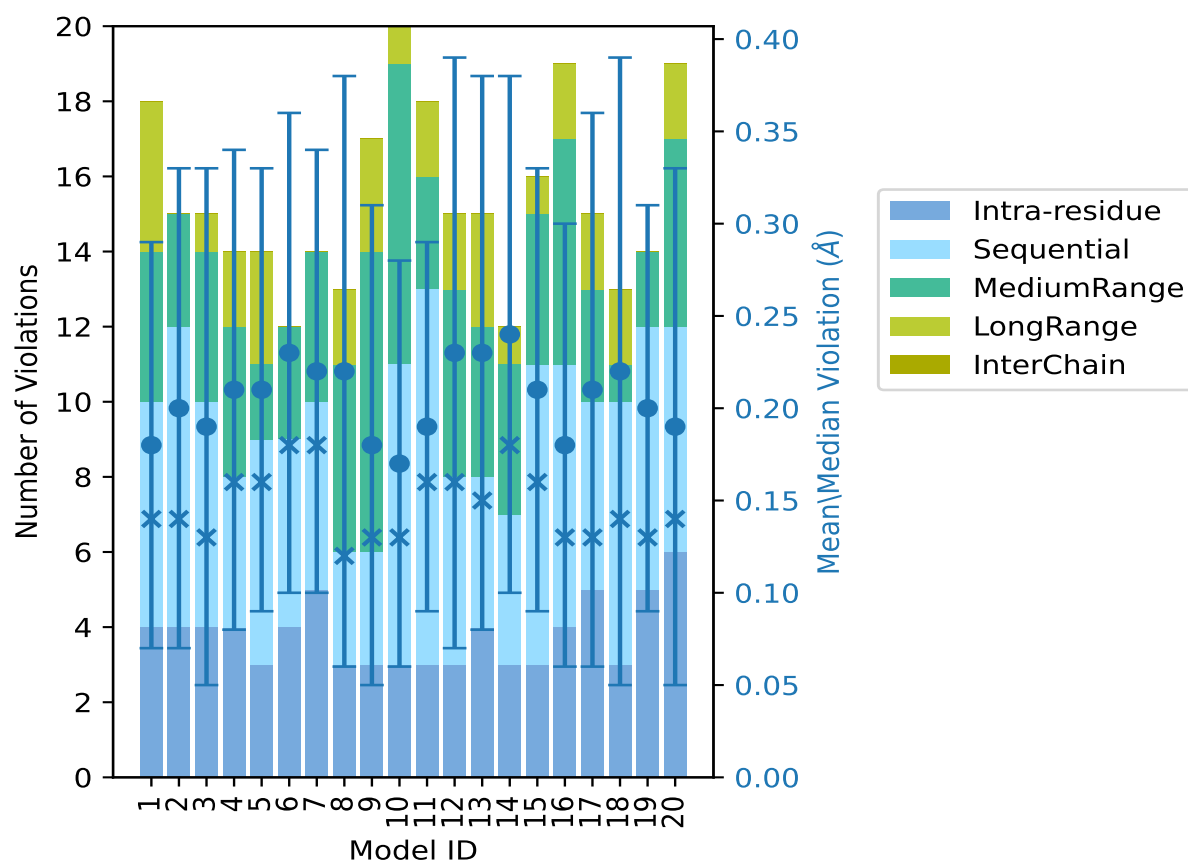
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 3                    | 10              | 3               | 2               | 0               | 18    | 0.19     | 0.55    | 0.1                 | 0.16       |
| 12       | 3                    | 5               | 5               | 2               | 0               | 15    | 0.23     | 0.63    | 0.16                | 0.16       |
| 13       | 4                    | 4               | 4               | 3               | 0               | 15    | 0.23     | 0.6     | 0.15                | 0.15       |
| 14       | 3                    | 4               | 4               | 1               | 0               | 12    | 0.24     | 0.62    | 0.14                | 0.18       |
| 15       | 3                    | 8               | 4               | 1               | 0               | 16    | 0.21     | 0.59    | 0.12                | 0.16       |
| 16       | 4                    | 7               | 6               | 2               | 0               | 19    | 0.18     | 0.58    | 0.12                | 0.13       |
| 17       | 5                    | 5               | 3               | 2               | 0               | 15    | 0.21     | 0.57    | 0.15                | 0.13       |
| 18       | 3                    | 7               | 1               | 2               | 0               | 13    | 0.22     | 0.64    | 0.17                | 0.14       |
| 19       | 5                    | 7               | 2               | 0               | 0               | 14    | 0.2      | 0.45    | 0.11                | 0.13       |
| 20       | 6                    | 6               | 5               | 2               | 0               | 19    | 0.19     | 0.63    | 0.14                | 0.14       |

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

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

### 9.3 Distance violation statistics for the ensemble

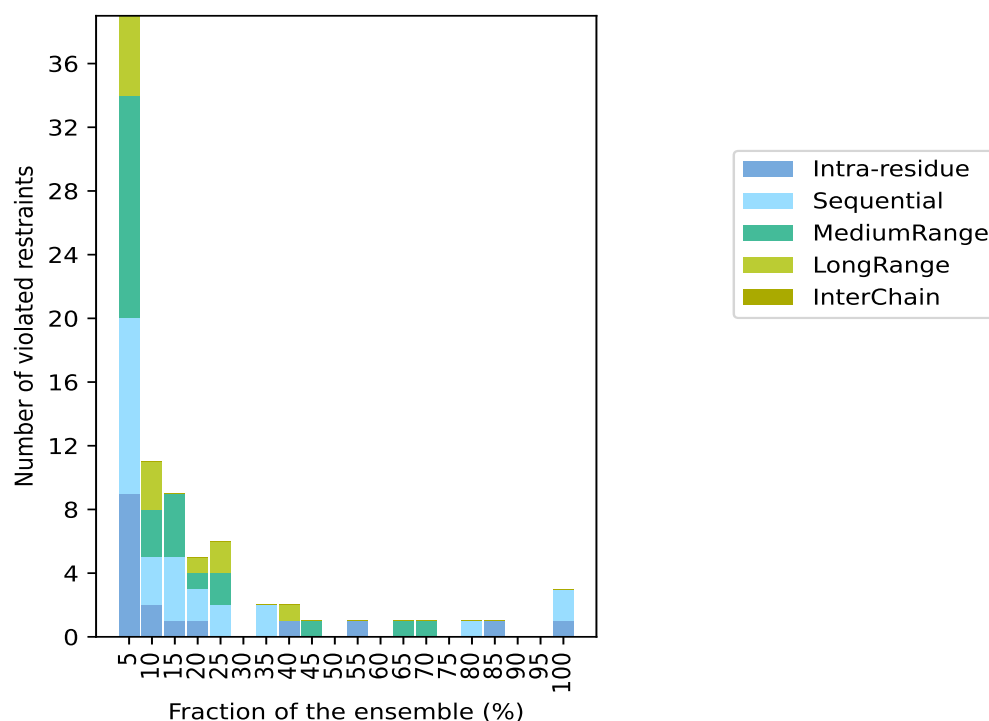
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3816(IR:991, SQ:962, MR:970, LR:893, IC:0) restraints are 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>       | %     |
| 9                             | 11              | 14              | 5               | 0               | 39    | 1                        | 5.0   |
| 2                             | 3               | 3               | 3               | 0               | 11    | 2                        | 10.0  |
| 1                             | 4               | 4               | 0               | 0               | 9     | 3                        | 15.0  |
| 1                             | 2               | 1               | 1               | 0               | 5     | 4                        | 20.0  |
| 0                             | 2               | 2               | 2               | 0               | 6     | 5                        | 25.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 6                        | 30.0  |
| 0                             | 2               | 0               | 0               | 0               | 2     | 7                        | 35.0  |
| 1                             | 0               | 0               | 1               | 0               | 2     | 8                        | 40.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 9                        | 45.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 10                       | 50.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 11                       | 55.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 12                       | 60.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 13                       | 65.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 14                       | 70.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 15                       | 75.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 16                       | 80.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 17                       | 85.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 18                       | 90.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 19                       | 95.0  |
| 1                             | 2               | 0               | 0               | 0               | 3     | 20                       | 100.0 |

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

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

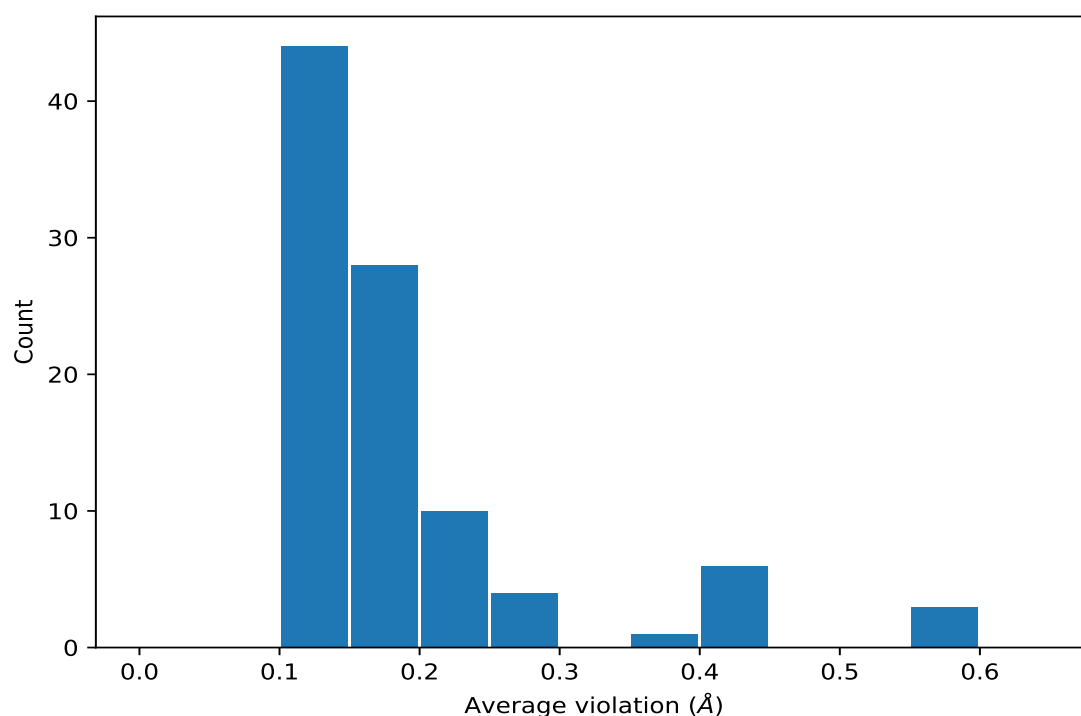
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 20                  | 0.56     | 0.09                | 0.58       |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 20                  | 0.56     | 0.09                | 0.58       |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 20                  | 0.56     | 0.09                | 0.58       |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H   | 20                  | 0.36     | 0.06                | 0.38       |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 20                  | 0.21     | 0.01                | 0.21       |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 17                  | 0.15     | 0.02                | 0.15       |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 16                  | 0.13     | 0.01                | 0.13       |
| (1,875)  | 1:69:A:LEU:H     | 1:71:A:LEU:HB2  | 14                  | 0.13     | 0.01                | 0.14       |
| (1,802)  | 1:121:A:VAL:HB   | 1:123:A:ASP:H   | 13                  | 0.13     | 0.02                | 0.13       |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD11 | 11                  | 0.27     | 0.07                | 0.29       |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD12 | 11                  | 0.27     | 0.07                | 0.29       |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD13 | 11                  | 0.27     | 0.07                | 0.29       |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB2  | 9                   | 0.13     | 0.02                | 0.12       |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB3  | 9                   | 0.13     | 0.02                | 0.12       |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB2  | 9                   | 0.13     | 0.02                | 0.12       |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB3  | 9                   | 0.13     | 0.02                | 0.12       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD11 | 8                   | 0.4      | 0.21                | 0.55       |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD12 | 8                   | 0.4      | 0.21                | 0.55       |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD13 | 8                   | 0.4      | 0.21                | 0.55       |
| (1,370)  | 1:129:A:SER:H    | 1:142:A:ALA:HB1 | 8                   | 0.13     | 0.01                | 0.12       |
| (1,370)  | 1:129:A:SER:H    | 1:142:A:ALA:HB2 | 8                   | 0.13     | 0.01                | 0.12       |
| (1,370)  | 1:129:A:SER:H    | 1:142:A:ALA:HB3 | 8                   | 0.13     | 0.01                | 0.12       |
| (1,1981) | 1:474:A:VAL:HG21 | 1:475:A:LEU:H   | 7                   | 0.14     | 0.01                | 0.14       |
| (1,1981) | 1:474:A:VAL:HG22 | 1:475:A:LEU:H   | 7                   | 0.14     | 0.01                | 0.14       |
| (1,1981) | 1:474:A:VAL:HG23 | 1:475:A:LEU:H   | 7                   | 0.14     | 0.01                | 0.14       |
| (1,2933) | 1:473:A:SER:HB2  | 1:474:A:VAL:HB  | 7                   | 0.14     | 0.03                | 0.13       |
| (1,2933) | 1:473:A:SER:HB3  | 1:474:A:VAL:HB  | 7                   | 0.14     | 0.03                | 0.13       |
| (1,2268) | 1:85:A:LEU:HG    | 1:140:A:PHE:HD1 | 5                   | 0.17     | 0.03                | 0.17       |
| (1,2268) | 1:85:A:LEU:HG    | 1:140:A:PHE:HD2 | 5                   | 0.17     | 0.03                | 0.17       |
| (1,451)  | 1:473:A:SER:HA   | 1:474:A:VAL:H   | 5                   | 0.16     | 0.03                | 0.16       |
| (1,166)  | 1:66:A:SER:H     | 1:69:A:LEU:HG   | 5                   | 0.13     | 0.01                | 0.12       |
| (1,911)  | 1:89:A:PHE:H     | 1:140:A:PHE:HD1 | 5                   | 0.12     | 0.01                | 0.12       |
| (1,911)  | 1:89:A:PHE:H     | 1:140:A:PHE:HD2 | 5                   | 0.12     | 0.01                | 0.12       |
| (1,289)  | 1:135:A:ILE:H    | 1:139:A:GLN:HB3 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,129)  | 1:98:A:GLY:H     | 1:99:A:LEU:HB2  | 5                   | 0.1      | 0.0                 | 0.1        |
| (1,2139) | 1:85:A:LEU:H     | 1:85:A:LEU:HD21 | 4                   | 0.43     | 0.04                | 0.44       |
| (1,2139) | 1:85:A:LEU:H     | 1:85:A:LEU:HD22 | 4                   | 0.43     | 0.04                | 0.44       |
| (1,2139) | 1:85:A:LEU:H     | 1:85:A:LEU:HD23 | 4                   | 0.43     | 0.04                | 0.44       |
| (1,1459) | 1:145:A:SER:HA   | 1:146:A:LYS:H   | 4                   | 0.22     | 0.04                | 0.23       |
| (1,162)  | 1:112:A:ILE:H    | 1:113:A:GLY:HA3 | 4                   | 0.19     | 0.09                | 0.18       |
| (1,3459) | 1:76:A:LEU:HD11  | 1:81:A:SER:HB2  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,3459) | 1:76:A:LEU:HD11  | 1:81:A:SER:HB3  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,3459) | 1:76:A:LEU:HD12  | 1:81:A:SER:HB2  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,3459) | 1:76:A:LEU:HD12  | 1:81:A:SER:HB3  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,3459) | 1:76:A:LEU:HD13  | 1:81:A:SER:HB2  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,3459) | 1:76:A:LEU:HD13  | 1:81:A:SER:HB3  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,3459) | 1:76:A:LEU:HD21  | 1:81:A:SER:HB2  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,3459) | 1:76:A:LEU:HD21  | 1:81:A:SER:HB3  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,3459) | 1:76:A:LEU:HD22  | 1:81:A:SER:HB2  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,3459) | 1:76:A:LEU:HD22  | 1:81:A:SER:HB3  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,3459) | 1:76:A:LEU:HD23  | 1:81:A:SER:HB2  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,3459) | 1:76:A:LEU:HD23  | 1:81:A:SER:HB3  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,1297) | 1:67:A:GLU:HG3   | 1:70:A:ALA:H    | 4                   | 0.12     | 0.02                | 0.11       |
| (1,223)  | 1:5:A:THR:H      | 1:8:A:GLN:HA    | 3                   | 0.21     | 0.01                | 0.21       |
| (1,2572) | 1:57:A:VAL:HB    | 1:58:A:ASP:HA   | 3                   | 0.21     | 0.0                 | 0.21       |
| (1,611)  | 1:51:A:LEU:HG    | 1:52:A:MET:H    | 3                   | 0.17     | 0.01                | 0.16       |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG11 | 3                   | 0.16     | 0.02                | 0.17       |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG12 | 3                   | 0.16     | 0.02                | 0.17       |

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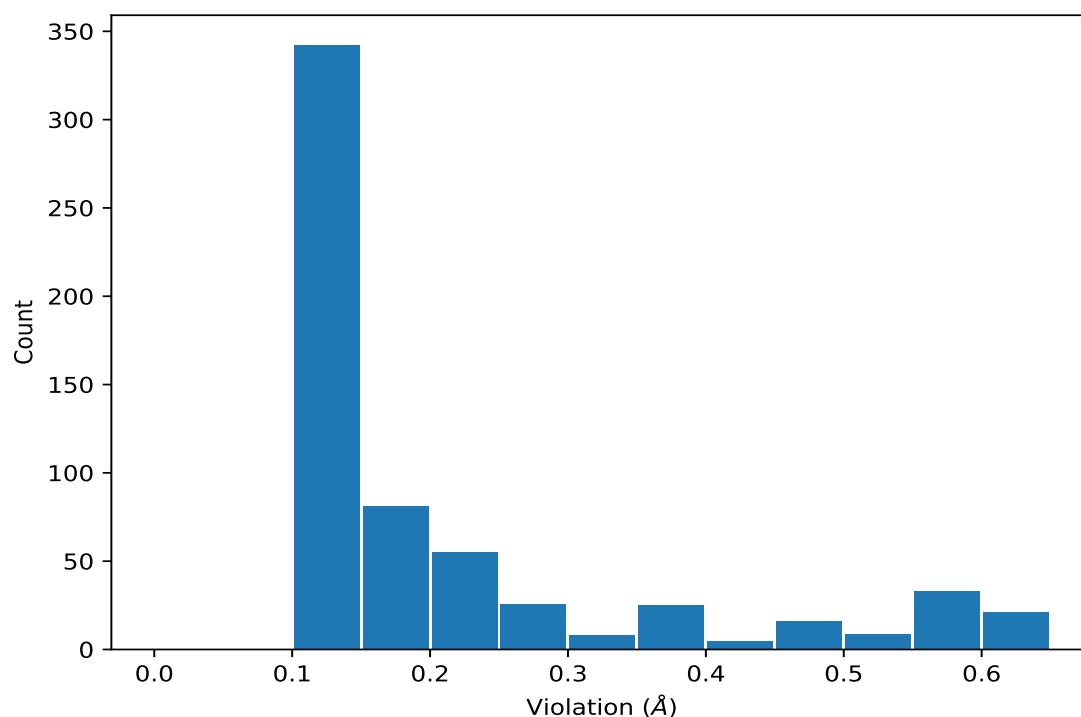
| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG13 | 3                   | 0.16     | 0.02                | 0.17       |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG21 | 3                   | 0.16     | 0.02                | 0.17       |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG22 | 3                   | 0.16     | 0.02                | 0.17       |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG23 | 3                   | 0.16     | 0.02                | 0.17       |
| (1,1268) | 1:4:A:LEU:H      | 1:8:A:GLN:HG3   | 3                   | 0.16     | 0.02                | 0.15       |
| (1,2059) | 1:91:A:VAL:HG21  | 1:92:A:PHE:HD1  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,2059) | 1:91:A:VAL:HG21  | 1:92:A:PHE:HD2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,2059) | 1:91:A:VAL:HG22  | 1:92:A:PHE:HD1  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,2059) | 1:91:A:VAL:HG22  | 1:92:A:PHE:HD2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,2059) | 1:91:A:VAL:HG23  | 1:92:A:PHE:HD1  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,2059) | 1:91:A:VAL:HG23  | 1:92:A:PHE:HD2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,2260) | 1:476:A:ARG:H    | 1:476:A:ARG:HG2 | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,817)  | 1:68:A:PHE:HB2   | 1:71:A:LEU:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,60)   | 1:94:A:LYS:HG2   | 1:96:A:GLY:H    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,60)   | 1:94:A:LYS:HG3   | 1:96:A:GLY:H    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,2779) | 1:126:A:ARG:HA   | 1:131:A:GLY:HA3 | 2                   | 0.3      | 0.18                | 0.3        |
| (1,3591) | 1:105:A:LEU:HD11 | 1:106:A:LYS:HA  | 2                   | 0.21     | 0.03                | 0.21       |
| (1,3591) | 1:105:A:LEU:HD12 | 1:106:A:LYS:HA  | 2                   | 0.21     | 0.03                | 0.21       |
| (1,3591) | 1:105:A:LEU:HD13 | 1:106:A:LYS:HA  | 2                   | 0.21     | 0.03                | 0.21       |
| (1,3591) | 1:105:A:LEU:HD21 | 1:106:A:LYS:HA  | 2                   | 0.21     | 0.03                | 0.21       |
| (1,3591) | 1:105:A:LEU:HD22 | 1:106:A:LYS:HA  | 2                   | 0.21     | 0.03                | 0.21       |
| (1,3591) | 1:105:A:LEU:HD23 | 1:106:A:LYS:HA  | 2                   | 0.21     | 0.03                | 0.21       |
| (1,812)  | 1:71:A:LEU:H     | 1:72:A:MET:HB2  | 2                   | 0.17     | 0.02                | 0.17       |
| (1,812)  | 1:71:A:LEU:H     | 1:72:A:MET:HB3  | 2                   | 0.17     | 0.02                | 0.17       |
| (1,649)  | 1:467:A:LYS:H    | 1:467:A:LYS:HD2 | 2                   | 0.16     | 0.01                | 0.16       |
| (1,649)  | 1:467:A:LYS:H    | 1:467:A:LYS:HD3 | 2                   | 0.16     | 0.01                | 0.16       |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD11 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD12 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD13 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD21 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD22 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD23 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,1409) | 1:102:A:ALA:H    | 1:105:A:LEU:HB2 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,179)  | 1:66:A:SER:H     | 1:70:A:ALA:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1081) | 1:144:A:LEU:HA   | 1:459:A:ARG:HE  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1610) | 1:57:A:VAL:H     | 1:67:A:GLU:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,513)  | 1:80:A:ASP:H     | 1:81:A:SER:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1637) | 1:64:A:GLU:H     | 1:68:A:PHE:HA   | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 18       | 0.64          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 18       | 0.64          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 18       | 0.64          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 3        | 0.63          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 3        | 0.63          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 3        | 0.63          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 9        | 0.63          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 9        | 0.63          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 9        | 0.63          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 12       | 0.63          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 12       | 0.63          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 12       | 0.63          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 20       | 0.63          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 20       | 0.63          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 20       | 0.63          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 2        | 0.62          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 2        | 0.62          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 2        | 0.62          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 14       | 0.62          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 14       | 0.62          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 14       | 0.62          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 13       | 0.6           |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 13       | 0.6           |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 13       | 0.6           |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 15       | 0.59          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 15       | 0.59          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 15       | 0.59          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 8        | 0.58          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 8        | 0.58          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 8        | 0.58          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 16       | 0.58          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 16       | 0.58          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 16       | 0.58          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD11 | 17       | 0.57          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD12 | 17       | 0.57          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD13 | 17       | 0.57          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 4        | 0.57          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 4        | 0.57          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 4        | 0.57          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 10       | 0.57          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 10       | 0.57          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 10       | 0.57          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD11 | 13       | 0.56          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD12 | 13       | 0.56          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD13 | 13       | 0.56          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD11 | 5        | 0.55          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD12 | 5        | 0.55          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD13 | 5        | 0.55          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD11 | 18       | 0.55          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD12 | 18       | 0.55          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD13 | 18       | 0.55          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 11       | 0.55          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 11       | 0.55          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 11       | 0.55          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD11 | 8        | 0.54          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD12 | 8        | 0.54          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD13 | 8        | 0.54          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 1        | 0.53          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 1        | 0.53          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 1        | 0.53          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 17       | 0.52          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 17       | 0.52          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 17       | 0.52          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 6        | 0.49          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 6        | 0.49          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 6        | 0.49          |
| (1,2779) | 1:126:A:ARG:HA   | 1:131:A:GLY:HA3 | 12       | 0.48          |
| (1,2139) | 1:85:A:LEU:H     | 1:85:A:LEU:HD21 | 20       | 0.48          |
| (1,2139) | 1:85:A:LEU:H     | 1:85:A:LEU:HD22 | 20       | 0.48          |
| (1,2139) | 1:85:A:LEU:H     | 1:85:A:LEU:HD23 | 20       | 0.48          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 7        | 0.48          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 7        | 0.48          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 7        | 0.48          |
| (1,2139) | 1:85:A:LEU:H     | 1:85:A:LEU:HD21 | 6        | 0.46          |
| (1,2139) | 1:85:A:LEU:H     | 1:85:A:LEU:HD22 | 6        | 0.46          |
| (1,2139) | 1:85:A:LEU:H     | 1:85:A:LEU:HD23 | 6        | 0.46          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 19       | 0.45          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 19       | 0.45          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 19       | 0.45          |
| (1,2139) | 1:85:A:LEU:H     | 1:85:A:LEU:HD21 | 7        | 0.42          |
| (1,2139) | 1:85:A:LEU:H     | 1:85:A:LEU:HD22 | 7        | 0.42          |
| (1,2139) | 1:85:A:LEU:H     | 1:85:A:LEU:HD23 | 7        | 0.42          |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H   | 5        | 0.4           |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H   | 16       | 0.4           |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H   | 9        | 0.39          |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H   | 12       | 0.39          |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H   | 19       | 0.39          |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H   | 3        | 0.38          |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H   | 4        | 0.38          |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H   | 7        | 0.38          |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H   | 13       | 0.38          |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H   | 14       | 0.38          |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H   | 15       | 0.38          |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H   | 17       | 0.38          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2139) | 1:85:A:LEU:H    | 1:85:A:LEU:HD21 | 4        | 0.37          |
| (1,2139) | 1:85:A:LEU:H    | 1:85:A:LEU:HD22 | 4        | 0.37          |
| (1,2139) | 1:85:A:LEU:H    | 1:85:A:LEU:HD23 | 4        | 0.37          |
| (1,1052) | 1:113:A:GLY:HA2 | 1:114:A:GLU:H   | 6        | 0.37          |
| (1,1052) | 1:113:A:GLY:HA2 | 1:114:A:GLU:H   | 18       | 0.37          |
| (1,1052) | 1:113:A:GLY:HA2 | 1:114:A:GLU:H   | 20       | 0.37          |
| (1,1052) | 1:113:A:GLY:HA2 | 1:114:A:GLU:H   | 2        | 0.36          |
| (1,1052) | 1:113:A:GLY:HA2 | 1:114:A:GLU:H   | 8        | 0.36          |
| (1,1052) | 1:113:A:GLY:HA2 | 1:114:A:GLU:H   | 11       | 0.36          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD11 | 12       | 0.36          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD12 | 12       | 0.36          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD13 | 12       | 0.36          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD11 | 14       | 0.36          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD12 | 14       | 0.36          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD13 | 14       | 0.36          |
| (1,1052) | 1:113:A:GLY:HA2 | 1:114:A:GLU:H   | 1        | 0.35          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD11 | 19       | 0.32          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD12 | 19       | 0.32          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD13 | 19       | 0.32          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD11 | 15       | 0.31          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD12 | 15       | 0.31          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD13 | 15       | 0.31          |
| (1,162)  | 1:112:A:ILE:H   | 1:113:A:GLY:HA3 | 10       | 0.31          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD11 | 2        | 0.3           |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD12 | 2        | 0.3           |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD13 | 2        | 0.3           |
| (1,3459) | 1:76:A:LEU:HD11 | 1:81:A:SER:HB2  | 1        | 0.29          |
| (1,3459) | 1:76:A:LEU:HD11 | 1:81:A:SER:HB3  | 1        | 0.29          |
| (1,3459) | 1:76:A:LEU:HD12 | 1:81:A:SER:HB2  | 1        | 0.29          |
| (1,3459) | 1:76:A:LEU:HD12 | 1:81:A:SER:HB3  | 1        | 0.29          |
| (1,3459) | 1:76:A:LEU:HD13 | 1:81:A:SER:HB2  | 1        | 0.29          |
| (1,3459) | 1:76:A:LEU:HD13 | 1:81:A:SER:HB3  | 1        | 0.29          |
| (1,3459) | 1:76:A:LEU:HD21 | 1:81:A:SER:HB2  | 1        | 0.29          |
| (1,3459) | 1:76:A:LEU:HD21 | 1:81:A:SER:HB3  | 1        | 0.29          |
| (1,3459) | 1:76:A:LEU:HD22 | 1:81:A:SER:HB2  | 1        | 0.29          |
| (1,3459) | 1:76:A:LEU:HD22 | 1:81:A:SER:HB3  | 1        | 0.29          |
| (1,3459) | 1:76:A:LEU:HD23 | 1:81:A:SER:HB2  | 1        | 0.29          |
| (1,3459) | 1:76:A:LEU:HD23 | 1:81:A:SER:HB3  | 1        | 0.29          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD11 | 3        | 0.29          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD12 | 3        | 0.29          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD13 | 3        | 0.29          |
| (1,1022) | 1:85:A:LEU:H    | 1:85:A:LEU:HD11 | 16       | 0.28          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD12 | 16       | 0.28          |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD13 | 16       | 0.28          |
| (1,1710) | 1:112:A:ILE:HD11 | 1:113:A:GLY:HA2 | 5        | 0.27          |
| (1,1710) | 1:112:A:ILE:HD12 | 1:113:A:GLY:HA2 | 5        | 0.27          |
| (1,1710) | 1:112:A:ILE:HD13 | 1:113:A:GLY:HA2 | 5        | 0.27          |
| (1,1459) | 1:145:A:SER:HA   | 1:146:A:LYS:H   | 2        | 0.26          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 10       | 0.25          |
| (1,3591) | 1:105:A:LEU:HD11 | 1:106:A:LYS:HA  | 14       | 0.24          |
| (1,3591) | 1:105:A:LEU:HD12 | 1:106:A:LYS:HA  | 14       | 0.24          |
| (1,3591) | 1:105:A:LEU:HD13 | 1:106:A:LYS:HA  | 14       | 0.24          |
| (1,3591) | 1:105:A:LEU:HD21 | 1:106:A:LYS:HA  | 14       | 0.24          |
| (1,3591) | 1:105:A:LEU:HD22 | 1:106:A:LYS:HA  | 14       | 0.24          |
| (1,3591) | 1:105:A:LEU:HD23 | 1:106:A:LYS:HA  | 14       | 0.24          |
| (1,1459) | 1:145:A:SER:HA   | 1:146:A:LYS:H   | 13       | 0.24          |
| (1,162)  | 1:112:A:ILE:H    | 1:113:A:GLY:HA3 | 7        | 0.24          |
| (1,3163) | 1:13:A:LYS:HB2   | 1:14:A:GLU:H    | 16       | 0.23          |
| (1,3163) | 1:13:A:LYS:HB3   | 1:14:A:GLU:H    | 16       | 0.23          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 1        | 0.23          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 7        | 0.23          |
| (1,2495) | 1:461:A:LYS:HB3  | 1:461:A:LYS:HE2 | 19       | 0.22          |
| (1,2495) | 1:461:A:LYS:HB3  | 1:461:A:LYS:HE3 | 19       | 0.22          |
| (1,2268) | 1:85:A:LEU:HG    | 1:140:A:PHE:HD1 | 13       | 0.22          |
| (1,2268) | 1:85:A:LEU:HG    | 1:140:A:PHE:HD2 | 13       | 0.22          |
| (1,1459) | 1:145:A:SER:HA   | 1:146:A:LYS:H   | 15       | 0.22          |
| (1,223)  | 1:5:A:THR:H      | 1:8:A:GLN:HA    | 14       | 0.22          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 8        | 0.22          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 11       | 0.22          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 12       | 0.22          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 17       | 0.22          |
| (1,3459) | 1:76:A:LEU:HD11  | 1:81:A:SER:HB2  | 20       | 0.21          |
| (1,3459) | 1:76:A:LEU:HD11  | 1:81:A:SER:HB3  | 20       | 0.21          |
| (1,3459) | 1:76:A:LEU:HD12  | 1:81:A:SER:HB2  | 20       | 0.21          |
| (1,3459) | 1:76:A:LEU:HD12  | 1:81:A:SER:HB3  | 20       | 0.21          |
| (1,3459) | 1:76:A:LEU:HD13  | 1:81:A:SER:HB2  | 20       | 0.21          |
| (1,3459) | 1:76:A:LEU:HD13  | 1:81:A:SER:HB3  | 20       | 0.21          |
| (1,3459) | 1:76:A:LEU:HD21  | 1:81:A:SER:HB2  | 20       | 0.21          |
| (1,3459) | 1:76:A:LEU:HD21  | 1:81:A:SER:HB3  | 20       | 0.21          |
| (1,3459) | 1:76:A:LEU:HD22  | 1:81:A:SER:HB2  | 20       | 0.21          |
| (1,3459) | 1:76:A:LEU:HD22  | 1:81:A:SER:HB3  | 20       | 0.21          |
| (1,3459) | 1:76:A:LEU:HD23  | 1:81:A:SER:HB2  | 20       | 0.21          |
| (1,3459) | 1:76:A:LEU:HD23  | 1:81:A:SER:HB3  | 20       | 0.21          |
| (1,2572) | 1:57:A:VAL:HB    | 1:58:A:ASP:HA   | 5        | 0.21          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2572) | 1:57:A:VAL:HB    | 1:58:A:ASP:HA   | 10       | 0.21          |
| (1,2572) | 1:57:A:VAL:HB    | 1:58:A:ASP:HA   | 11       | 0.21          |
| (1,223)  | 1:5:A:THR:H      | 1:8:A:GLN:HA    | 6        | 0.21          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 2        | 0.21          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 5        | 0.21          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 9        | 0.21          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 13       | 0.21          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 15       | 0.21          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 16       | 0.21          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 18       | 0.21          |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 20       | 0.21          |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD11 | 9        | 0.2           |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD12 | 9        | 0.2           |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD13 | 9        | 0.2           |
| (1,223)  | 1:5:A:THR:H      | 1:8:A:GLN:HA    | 7        | 0.2           |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 3        | 0.2           |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 4        | 0.2           |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 6        | 0.2           |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 14       | 0.2           |
| (1,45)   | 1:113:A:GLY:H    | 1:113:A:GLY:HA3 | 19       | 0.2           |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD11 | 7        | 0.19          |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD12 | 7        | 0.19          |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD13 | 7        | 0.19          |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD21 | 7        | 0.19          |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD22 | 7        | 0.19          |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD23 | 7        | 0.19          |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD11 | 1        | 0.19          |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD12 | 1        | 0.19          |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD13 | 1        | 0.19          |
| (1,812)  | 1:71:A:LEU:H     | 1:72:A:MET:HB2  | 11       | 0.19          |
| (1,812)  | 1:71:A:LEU:H     | 1:72:A:MET:HB3  | 11       | 0.19          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 8        | 0.19          |
| (1,451)  | 1:473:A:SER:HA   | 1:474:A:VAL:H   | 15       | 0.19          |
| (1,3591) | 1:105:A:LEU:HD11 | 1:106:A:LYS:HA  | 10       | 0.18          |
| (1,3591) | 1:105:A:LEU:HD12 | 1:106:A:LYS:HA  | 10       | 0.18          |
| (1,3591) | 1:105:A:LEU:HD13 | 1:106:A:LYS:HA  | 10       | 0.18          |
| (1,3591) | 1:105:A:LEU:HD21 | 1:106:A:LYS:HA  | 10       | 0.18          |
| (1,3591) | 1:105:A:LEU:HD22 | 1:106:A:LYS:HA  | 10       | 0.18          |
| (1,3591) | 1:105:A:LEU:HD23 | 1:106:A:LYS:HA  | 10       | 0.18          |
| (1,3494) | 1:85:A:LEU:HD11  | 1:89:A:PHE:H    | 4        | 0.18          |
| (1,3494) | 1:85:A:LEU:HD12  | 1:89:A:PHE:H    | 4        | 0.18          |
| (1,3494) | 1:85:A:LEU:HD13  | 1:89:A:PHE:H    | 4        | 0.18          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3494) | 1:85:A:LEU:HD21  | 1:89:A:PHE:H    | 4        | 0.18          |
| (1,3494) | 1:85:A:LEU:HD22  | 1:89:A:PHE:H    | 4        | 0.18          |
| (1,3494) | 1:85:A:LEU:HD23  | 1:89:A:PHE:H    | 4        | 0.18          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG11 | 11       | 0.18          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG12 | 11       | 0.18          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG13 | 11       | 0.18          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG21 | 11       | 0.18          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG22 | 11       | 0.18          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG23 | 11       | 0.18          |
| (1,2933) | 1:473:A:SER:HB2  | 1:474:A:VAL:HB  | 15       | 0.18          |
| (1,2933) | 1:473:A:SER:HB3  | 1:474:A:VAL:HB  | 15       | 0.18          |
| (1,1268) | 1:4:A:LEU:H      | 1:8:A:GLN:HG3   | 6        | 0.18          |
| (1,611)  | 1:51:A:LEU:HG    | 1:52:A:MET:H    | 3        | 0.18          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 17       | 0.18          |
| (1,425)  | 1:460:A:ASN:H    | 1:461:A:LYS:HB3 | 19       | 0.18          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG11 | 5        | 0.17          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG12 | 5        | 0.17          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG13 | 5        | 0.17          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG21 | 5        | 0.17          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG22 | 5        | 0.17          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG23 | 5        | 0.17          |
| (1,3140) | 1:9:A:ILE:HG21   | 1:13:A:LYS:HE2  | 16       | 0.17          |
| (1,3140) | 1:9:A:ILE:HG21   | 1:13:A:LYS:HE3  | 16       | 0.17          |
| (1,3140) | 1:9:A:ILE:HG22   | 1:13:A:LYS:HE2  | 16       | 0.17          |
| (1,3140) | 1:9:A:ILE:HG22   | 1:13:A:LYS:HE3  | 16       | 0.17          |
| (1,3140) | 1:9:A:ILE:HG23   | 1:13:A:LYS:HE2  | 16       | 0.17          |
| (1,3140) | 1:9:A:ILE:HG23   | 1:13:A:LYS:HE3  | 16       | 0.17          |
| (1,2933) | 1:473:A:SER:HB2  | 1:474:A:VAL:HB  | 11       | 0.17          |
| (1,2933) | 1:473:A:SER:HB3  | 1:474:A:VAL:HB  | 11       | 0.17          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB2  | 11       | 0.17          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB3  | 11       | 0.17          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB2  | 11       | 0.17          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB3  | 11       | 0.17          |
| (1,2268) | 1:85:A:LEU:HG    | 1:140:A:PHE:HD1 | 5        | 0.17          |
| (1,2268) | 1:85:A:LEU:HG    | 1:140:A:PHE:HD2 | 5        | 0.17          |
| (1,2268) | 1:85:A:LEU:HG    | 1:140:A:PHE:HD1 | 17       | 0.17          |
| (1,2268) | 1:85:A:LEU:HG    | 1:140:A:PHE:HD2 | 17       | 0.17          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 6        | 0.17          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 7        | 0.17          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 15       | 0.17          |
| (1,451)  | 1:473:A:SER:HA   | 1:474:A:VAL:H   | 20       | 0.17          |
| (1,1981) | 1:474:A:VAL:HG21 | 1:475:A:LEU:H   | 1        | 0.16          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1981) | 1:474:A:VAL:HG22 | 1:475:A:LEU:H   | 1        | 0.16          |
| (1,1981) | 1:474:A:VAL:HG23 | 1:475:A:LEU:H   | 1        | 0.16          |
| (1,1981) | 1:474:A:VAL:HG21 | 1:475:A:LEU:H   | 6        | 0.16          |
| (1,1981) | 1:474:A:VAL:HG22 | 1:475:A:LEU:H   | 6        | 0.16          |
| (1,1981) | 1:474:A:VAL:HG23 | 1:475:A:LEU:H   | 6        | 0.16          |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD11 | 10       | 0.16          |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD12 | 10       | 0.16          |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD13 | 10       | 0.16          |
| (1,802)  | 1:121:A:VAL:HB   | 1:123:A:ASP:H   | 11       | 0.16          |
| (1,802)  | 1:121:A:VAL:HB   | 1:123:A:ASP:H   | 12       | 0.16          |
| (1,649)  | 1:467:A:LYS:H    | 1:467:A:LYS:HD2 | 2        | 0.16          |
| (1,649)  | 1:467:A:LYS:H    | 1:467:A:LYS:HD3 | 2        | 0.16          |
| (1,611)  | 1:51:A:LEU:HG    | 1:52:A:MET:H    | 4        | 0.16          |
| (1,611)  | 1:51:A:LEU:HG    | 1:52:A:MET:H    | 12       | 0.16          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 4        | 0.16          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 12       | 0.16          |
| (1,451)  | 1:473:A:SER:HA   | 1:474:A:VAL:H   | 11       | 0.16          |
| (1,2854) | 1:13:A:LYS:HA    | 1:13:A:LYS:HG2  | 16       | 0.15          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB2  | 10       | 0.15          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB3  | 10       | 0.15          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB2  | 10       | 0.15          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB3  | 10       | 0.15          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD11 | 4        | 0.15          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD12 | 4        | 0.15          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD13 | 4        | 0.15          |
| (1,2059) | 1:91:A:VAL:HG21  | 1:92:A:PHE:HD1  | 5        | 0.15          |
| (1,2059) | 1:91:A:VAL:HG21  | 1:92:A:PHE:HD2  | 5        | 0.15          |
| (1,2059) | 1:91:A:VAL:HG22  | 1:92:A:PHE:HD1  | 5        | 0.15          |
| (1,2059) | 1:91:A:VAL:HG22  | 1:92:A:PHE:HD2  | 5        | 0.15          |
| (1,2059) | 1:91:A:VAL:HG23  | 1:92:A:PHE:HD1  | 5        | 0.15          |
| (1,2059) | 1:91:A:VAL:HG23  | 1:92:A:PHE:HD2  | 5        | 0.15          |
| (1,1459) | 1:145:A:SER:HA   | 1:146:A:LYS:H   | 16       | 0.15          |
| (1,1297) | 1:67:A:GLU:HG3   | 1:70:A:ALA:H    | 20       | 0.15          |
| (1,1268) | 1:4:A:LEU:H      | 1:8:A:GLN:HG3   | 7        | 0.15          |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD11 | 11       | 0.15          |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD12 | 11       | 0.15          |
| (1,1022) | 1:85:A:LEU:H     | 1:85:A:LEU:HD13 | 11       | 0.15          |
| (1,875)  | 1:69:A:LEU:H     | 1:71:A:LEU:HB2  | 1        | 0.15          |
| (1,875)  | 1:69:A:LEU:H     | 1:71:A:LEU:HB2  | 9        | 0.15          |
| (1,875)  | 1:69:A:LEU:H     | 1:71:A:LEU:HB2  | 13       | 0.15          |
| (1,812)  | 1:71:A:LEU:H     | 1:72:A:MET:HB2  | 7        | 0.15          |
| (1,812)  | 1:71:A:LEU:H     | 1:72:A:MET:HB3  | 7        | 0.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,802)  | 1:121:A:VAL:HB   | 1:123:A:ASP:H   | 15       | 0.15          |
| (1,649)  | 1:467:A:LYS:H    | 1:467:A:LYS:HD2 | 13       | 0.15          |
| (1,649)  | 1:467:A:LYS:H    | 1:467:A:LYS:HD3 | 13       | 0.15          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 1        | 0.15          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 13       | 0.15          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 14       | 0.15          |
| (1,451)  | 1:473:A:SER:HA   | 1:474:A:VAL:H   | 18       | 0.15          |
| (1,370)  | 1:129:A:SER:H    | 1:142:A:ALA:HB1 | 13       | 0.15          |
| (1,370)  | 1:129:A:SER:H    | 1:142:A:ALA:HB2 | 13       | 0.15          |
| (1,370)  | 1:129:A:SER:H    | 1:142:A:ALA:HB3 | 13       | 0.15          |
| (1,166)  | 1:66:A:SER:H     | 1:69:A:LEU:HG   | 9        | 0.15          |
| (1,3459) | 1:76:A:LEU:HD11  | 1:81:A:SER:HB2  | 15       | 0.14          |
| (1,3459) | 1:76:A:LEU:HD11  | 1:81:A:SER:HB3  | 15       | 0.14          |
| (1,3459) | 1:76:A:LEU:HD12  | 1:81:A:SER:HB2  | 15       | 0.14          |
| (1,3459) | 1:76:A:LEU:HD12  | 1:81:A:SER:HB3  | 15       | 0.14          |
| (1,3459) | 1:76:A:LEU:HD13  | 1:81:A:SER:HB2  | 15       | 0.14          |
| (1,3459) | 1:76:A:LEU:HD13  | 1:81:A:SER:HB3  | 15       | 0.14          |
| (1,3459) | 1:76:A:LEU:HD21  | 1:81:A:SER:HB2  | 15       | 0.14          |
| (1,3459) | 1:76:A:LEU:HD21  | 1:81:A:SER:HB3  | 15       | 0.14          |
| (1,3459) | 1:76:A:LEU:HD22  | 1:81:A:SER:HB2  | 15       | 0.14          |
| (1,3459) | 1:76:A:LEU:HD22  | 1:81:A:SER:HB3  | 15       | 0.14          |
| (1,3459) | 1:76:A:LEU:HD23  | 1:81:A:SER:HB2  | 15       | 0.14          |
| (1,3459) | 1:76:A:LEU:HD23  | 1:81:A:SER:HB3  | 15       | 0.14          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG11 | 10       | 0.14          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG12 | 10       | 0.14          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG13 | 10       | 0.14          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG21 | 10       | 0.14          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG22 | 10       | 0.14          |
| (1,3371) | 1:56:A:ASP:H     | 1:57:A:VAL:HG23 | 10       | 0.14          |
| (1,2933) | 1:473:A:SER:HB2  | 1:474:A:VAL:HB  | 18       | 0.14          |
| (1,2933) | 1:473:A:SER:HB3  | 1:474:A:VAL:HB  | 18       | 0.14          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB2  | 12       | 0.14          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB3  | 12       | 0.14          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB2  | 12       | 0.14          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB3  | 12       | 0.14          |
| (1,2268) | 1:85:A:LEU:HG    | 1:140:A:PHE:HD1 | 8        | 0.14          |
| (1,2268) | 1:85:A:LEU:HG    | 1:140:A:PHE:HD2 | 8        | 0.14          |
| (1,1981) | 1:474:A:VAL:HG21 | 1:475:A:LEU:H   | 2        | 0.14          |
| (1,1981) | 1:474:A:VAL:HG22 | 1:475:A:LEU:H   | 2        | 0.14          |
| (1,1981) | 1:474:A:VAL:HG23 | 1:475:A:LEU:H   | 2        | 0.14          |
| (1,1981) | 1:474:A:VAL:HG21 | 1:475:A:LEU:H   | 15       | 0.14          |
| (1,1981) | 1:474:A:VAL:HG22 | 1:475:A:LEU:H   | 15       | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1981) | 1:474:A:VAL:HG23 | 1:475:A:LEU:H   | 15       | 0.14          |
| (1,1981) | 1:474:A:VAL:HG21 | 1:475:A:LEU:H   | 18       | 0.14          |
| (1,1981) | 1:474:A:VAL:HG22 | 1:475:A:LEU:H   | 18       | 0.14          |
| (1,1981) | 1:474:A:VAL:HG23 | 1:475:A:LEU:H   | 18       | 0.14          |
| (1,1981) | 1:474:A:VAL:HG21 | 1:475:A:LEU:H   | 20       | 0.14          |
| (1,1981) | 1:474:A:VAL:HG22 | 1:475:A:LEU:H   | 20       | 0.14          |
| (1,1981) | 1:474:A:VAL:HG23 | 1:475:A:LEU:H   | 20       | 0.14          |
| (1,1409) | 1:102:A:ALA:H    | 1:105:A:LEU:HB2 | 14       | 0.14          |
| (1,1268) | 1:4:A:LEU:H      | 1:8:A:GLN:HG3   | 14       | 0.14          |
| (1,911)  | 1:89:A:PHE:H     | 1:140:A:PHE:HD1 | 13       | 0.14          |
| (1,911)  | 1:89:A:PHE:H     | 1:140:A:PHE:HD2 | 13       | 0.14          |
| (1,875)  | 1:69:A:LEU:H     | 1:71:A:LEU:HB2  | 4        | 0.14          |
| (1,875)  | 1:69:A:LEU:H     | 1:71:A:LEU:HB2  | 10       | 0.14          |
| (1,875)  | 1:69:A:LEU:H     | 1:71:A:LEU:HB2  | 15       | 0.14          |
| (1,875)  | 1:69:A:LEU:H     | 1:71:A:LEU:HB2  | 20       | 0.14          |
| (1,848)  | 1:86:A:LEU:H     | 1:87:A:GLU:HG2  | 15       | 0.14          |
| (1,802)  | 1:121:A:VAL:HB   | 1:123:A:ASP:H   | 16       | 0.14          |
| (1,697)  | 1:467:A:LYS:HD2  | 1:468:A:VAL:H   | 2        | 0.14          |
| (1,697)  | 1:467:A:LYS:HD3  | 1:468:A:VAL:H   | 2        | 0.14          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 3        | 0.14          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 20       | 0.14          |
| (1,370)  | 1:129:A:SER:H    | 1:142:A:ALA:HB1 | 1        | 0.14          |
| (1,370)  | 1:129:A:SER:H    | 1:142:A:ALA:HB2 | 1        | 0.14          |
| (1,370)  | 1:129:A:SER:H    | 1:142:A:ALA:HB3 | 1        | 0.14          |
| (1,2933) | 1:473:A:SER:HB2  | 1:474:A:VAL:HB  | 1        | 0.13          |
| (1,2933) | 1:473:A:SER:HB3  | 1:474:A:VAL:HB  | 1        | 0.13          |
| (1,2933) | 1:473:A:SER:HB2  | 1:474:A:VAL:HB  | 2        | 0.13          |
| (1,2933) | 1:473:A:SER:HB3  | 1:474:A:VAL:HB  | 2        | 0.13          |
| (1,2855) | 1:13:A:LYS:HA    | 1:13:A:LYS:HD2  | 16       | 0.13          |
| (1,2779) | 1:126:A:ARG:HA   | 1:131:A:GLY:HA3 | 1        | 0.13          |
| (1,2268) | 1:85:A:LEU:HG    | 1:140:A:PHE:HD1 | 18       | 0.13          |
| (1,2268) | 1:85:A:LEU:HG    | 1:140:A:PHE:HD2 | 18       | 0.13          |
| (1,2260) | 1:476:A:ARG:H    | 1:476:A:ARG:HG2 | 3        | 0.13          |
| (1,2260) | 1:476:A:ARG:H    | 1:476:A:ARG:HG2 | 5        | 0.13          |
| (1,2260) | 1:476:A:ARG:H    | 1:476:A:ARG:HG2 | 17       | 0.13          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD11 | 6        | 0.13          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD12 | 6        | 0.13          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD13 | 6        | 0.13          |
| (1,2137) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD21 | 7        | 0.13          |
| (1,2137) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD22 | 7        | 0.13          |
| (1,2137) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD23 | 7        | 0.13          |
| (1,2059) | 1:91:A:VAL:HG21  | 1:92:A:PHE:HD1  | 18       | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2059) | 1:91:A:VAL:HG21  | 1:92:A:PHE:HD2  | 18       | 0.13          |
| (1,2059) | 1:91:A:VAL:HG22  | 1:92:A:PHE:HD1  | 18       | 0.13          |
| (1,2059) | 1:91:A:VAL:HG22  | 1:92:A:PHE:HD2  | 18       | 0.13          |
| (1,2059) | 1:91:A:VAL:HG23  | 1:92:A:PHE:HD1  | 18       | 0.13          |
| (1,2059) | 1:91:A:VAL:HG23  | 1:92:A:PHE:HD2  | 18       | 0.13          |
| (1,1981) | 1:474:A:VAL:HG21 | 1:475:A:LEU:H   | 11       | 0.13          |
| (1,1981) | 1:474:A:VAL:HG22 | 1:475:A:LEU:H   | 11       | 0.13          |
| (1,1981) | 1:474:A:VAL:HG23 | 1:475:A:LEU:H   | 11       | 0.13          |
| (1,1409) | 1:102:A:ALA:H    | 1:105:A:LEU:HB2 | 10       | 0.13          |
| (1,1237) | 1:77:A:LYS:H     | 1:78:A:SER:H    | 19       | 0.13          |
| (1,1154) | 1:47:A:GLU:HB2   | 1:50:A:ASP:H    | 12       | 0.13          |
| (1,1053) | 1:114:A:GLU:H    | 1:115:A:LYS:HA  | 19       | 0.13          |
| (1,911)  | 1:89:A:PHE:H     | 1:140:A:PHE:HD1 | 5        | 0.13          |
| (1,911)  | 1:89:A:PHE:H     | 1:140:A:PHE:HD2 | 5        | 0.13          |
| (1,875)  | 1:69:A:LEU:H     | 1:71:A:LEU:HB2  | 6        | 0.13          |
| (1,875)  | 1:69:A:LEU:H     | 1:71:A:LEU:HB2  | 11       | 0.13          |
| (1,802)  | 1:121:A:VAL:HB   | 1:123:A:ASP:H   | 5        | 0.13          |
| (1,802)  | 1:121:A:VAL:HB   | 1:123:A:ASP:H   | 9        | 0.13          |
| (1,802)  | 1:121:A:VAL:HB   | 1:123:A:ASP:H   | 14       | 0.13          |
| (1,802)  | 1:121:A:VAL:HB   | 1:123:A:ASP:H   | 20       | 0.13          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 2        | 0.13          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 9        | 0.13          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 11       | 0.13          |
| (1,589)  | 1:61:A:HIS:H     | 1:61:A:HIS:HD2  | 18       | 0.13          |
| (1,515)  | 1:105:A:LEU:HD21 | 1:106:A:LYS:H   | 1        | 0.13          |
| (1,515)  | 1:105:A:LEU:HD22 | 1:106:A:LYS:H   | 1        | 0.13          |
| (1,515)  | 1:105:A:LEU:HD23 | 1:106:A:LYS:H   | 1        | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 1        | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 2        | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 3        | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 5        | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 6        | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 7        | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 10       | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 11       | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 13       | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 14       | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 16       | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 17       | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 19       | 0.13          |
| (1,461)  | 1:131:A:GLY:HA3  | 1:132:A:SER:H   | 20       | 0.13          |
| (1,370)  | 1:129:A:SER:H    | 1:142:A:ALA:HB1 | 16       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,370)  | 1:129:A:SER:H    | 1:142:A:ALA:HB2  | 16       | 0.13          |
| (1,370)  | 1:129:A:SER:H    | 1:142:A:ALA:HB3  | 16       | 0.13          |
| (1,289)  | 1:135:A:ILE:H    | 1:139:A:GLN:HB3  | 17       | 0.13          |
| (1,179)  | 1:66:A:SER:H     | 1:70:A:ALA:H     | 9        | 0.13          |
| (1,166)  | 1:66:A:SER:H     | 1:69:A:LEU:HG    | 12       | 0.13          |
| (1,2887) | 1:81:A:SER:HA    | 1:84:A:GLU:H     | 8        | 0.12          |
| (1,2793) | 1:90:A:LYS:HA    | 1:90:A:LYS:HG3   | 19       | 0.12          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB2   | 1        | 0.12          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB3   | 1        | 0.12          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB2   | 1        | 0.12          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB3   | 1        | 0.12          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB2   | 2        | 0.12          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB3   | 2        | 0.12          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB2   | 2        | 0.12          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB3   | 2        | 0.12          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB2   | 16       | 0.12          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB3   | 16       | 0.12          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB2   | 16       | 0.12          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB3   | 16       | 0.12          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB2   | 19       | 0.12          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB3   | 19       | 0.12          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB2   | 19       | 0.12          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB3   | 19       | 0.12          |
| (1,2328) | 1:90:A:LYS:HA    | 1:90:A:LYS:HD2   | 20       | 0.12          |
| (1,2328) | 1:90:A:LYS:HA    | 1:90:A:LYS:HD3   | 20       | 0.12          |
| (1,2187) | 1:85:A:LEU:HD11  | 1:141:A:ALA:H    | 4        | 0.12          |
| (1,2187) | 1:85:A:LEU:HD12  | 1:141:A:ALA:H    | 4        | 0.12          |
| (1,2187) | 1:85:A:LEU:HD13  | 1:141:A:ALA:H    | 4        | 0.12          |
| (1,2059) | 1:91:A:VAL:HG21  | 1:92:A:PHE:HD1   | 10       | 0.12          |
| (1,2059) | 1:91:A:VAL:HG21  | 1:92:A:PHE:HD2   | 10       | 0.12          |
| (1,2059) | 1:91:A:VAL:HG22  | 1:92:A:PHE:HD1   | 10       | 0.12          |
| (1,2059) | 1:91:A:VAL:HG22  | 1:92:A:PHE:HD2   | 10       | 0.12          |
| (1,2059) | 1:91:A:VAL:HG23  | 1:92:A:PHE:HD1   | 10       | 0.12          |
| (1,2059) | 1:91:A:VAL:HG23  | 1:92:A:PHE:HD2   | 10       | 0.12          |
| (1,1297) | 1:67:A:GLU:HG3   | 1:70:A:ALA:H     | 9        | 0.12          |
| (1,1215) | 1:130:A:ASP:H    | 1:139:A:GLN:HE22 | 12       | 0.12          |
| (1,1080) | 1:459:A:ARG:HA   | 1:459:A:ARG:HE   | 1        | 0.12          |
| (1,1066) | 1:100:A:ILE:HG21 | 1:104:A:GLU:H    | 4        | 0.12          |
| (1,1066) | 1:100:A:ILE:HG22 | 1:104:A:GLU:H    | 4        | 0.12          |
| (1,1066) | 1:100:A:ILE:HG23 | 1:104:A:GLU:H    | 4        | 0.12          |
| (1,1052) | 1:113:A:GLY:HA2  | 1:114:A:GLU:H    | 10       | 0.12          |
| (1,911)  | 1:89:A:PHE:H     | 1:140:A:PHE:HD1  | 17       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,911)  | 1:89:A:PHE:H    | 1:140:A:PHE:HD2 | 17       | 0.12          |
| (1,875)  | 1:69:A:LEU:H    | 1:71:A:LEU:HB2  | 2        | 0.12          |
| (1,875)  | 1:69:A:LEU:H    | 1:71:A:LEU:HB2  | 3        | 0.12          |
| (1,875)  | 1:69:A:LEU:H    | 1:71:A:LEU:HB2  | 17       | 0.12          |
| (1,817)  | 1:68:A:PHE:HB2  | 1:71:A:LEU:H    | 5        | 0.12          |
| (1,802)  | 1:121:A:VAL:HB  | 1:123:A:ASP:H   | 1        | 0.12          |
| (1,802)  | 1:121:A:VAL:HB  | 1:123:A:ASP:H   | 4        | 0.12          |
| (1,802)  | 1:121:A:VAL:HB  | 1:123:A:ASP:H   | 8        | 0.12          |
| (1,589)  | 1:61:A:HIS:H    | 1:61:A:HIS:HD2  | 19       | 0.12          |
| (1,461)  | 1:131:A:GLY:HA3 | 1:132:A:SER:H   | 15       | 0.12          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB1 | 3        | 0.12          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB2 | 3        | 0.12          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB3 | 3        | 0.12          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB1 | 5        | 0.12          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB2 | 5        | 0.12          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB3 | 5        | 0.12          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB1 | 11       | 0.12          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB2 | 11       | 0.12          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB3 | 11       | 0.12          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB1 | 20       | 0.12          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB2 | 20       | 0.12          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB3 | 20       | 0.12          |
| (1,289)  | 1:135:A:ILE:H   | 1:139:A:GLN:HB3 | 13       | 0.12          |
| (1,179)  | 1:66:A:SER:H    | 1:70:A:ALA:H    | 1        | 0.12          |
| (1,166)  | 1:66:A:SER:H    | 1:69:A:LEU:HG   | 10       | 0.12          |
| (1,166)  | 1:66:A:SER:H    | 1:69:A:LEU:HG   | 20       | 0.12          |
| (1,60)   | 1:94:A:LYS:HG2  | 1:96:A:GLY:H    | 20       | 0.12          |
| (1,60)   | 1:94:A:LYS:HG3  | 1:96:A:GLY:H    | 20       | 0.12          |
| (1,3849) | 1:467:A:LYS:H   | 1:467:A:LYS:HE2 | 17       | 0.11          |
| (1,3849) | 1:467:A:LYS:H   | 1:467:A:LYS:HE3 | 17       | 0.11          |
| (1,3459) | 1:76:A:LEU:HD11 | 1:81:A:SER:HB2  | 10       | 0.11          |
| (1,3459) | 1:76:A:LEU:HD11 | 1:81:A:SER:HB3  | 10       | 0.11          |
| (1,3459) | 1:76:A:LEU:HD12 | 1:81:A:SER:HB2  | 10       | 0.11          |
| (1,3459) | 1:76:A:LEU:HD12 | 1:81:A:SER:HB3  | 10       | 0.11          |
| (1,3459) | 1:76:A:LEU:HD13 | 1:81:A:SER:HB2  | 10       | 0.11          |
| (1,3459) | 1:76:A:LEU:HD13 | 1:81:A:SER:HB3  | 10       | 0.11          |
| (1,3459) | 1:76:A:LEU:HD21 | 1:81:A:SER:HB2  | 10       | 0.11          |
| (1,3459) | 1:76:A:LEU:HD21 | 1:81:A:SER:HB3  | 10       | 0.11          |
| (1,3459) | 1:76:A:LEU:HD22 | 1:81:A:SER:HB2  | 10       | 0.11          |
| (1,3459) | 1:76:A:LEU:HD22 | 1:81:A:SER:HB3  | 10       | 0.11          |
| (1,3459) | 1:76:A:LEU:HD23 | 1:81:A:SER:HB2  | 10       | 0.11          |
| (1,3459) | 1:76:A:LEU:HD23 | 1:81:A:SER:HB3  | 10       | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD11 | 10       | 0.11          |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD12 | 10       | 0.11          |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD13 | 10       | 0.11          |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD21 | 10       | 0.11          |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD22 | 10       | 0.11          |
| (1,3422) | 1:71:A:LEU:HA    | 1:71:A:LEU:HD23 | 10       | 0.11          |
| (1,2959) | 1:90:A:LYS:HD2   | 1:91:A:VAL:HA   | 19       | 0.11          |
| (1,2959) | 1:90:A:LYS:HD3   | 1:91:A:VAL:HA   | 19       | 0.11          |
| (1,2933) | 1:473:A:SER:HB2  | 1:474:A:VAL:HB  | 6        | 0.11          |
| (1,2933) | 1:473:A:SER:HB3  | 1:474:A:VAL:HB  | 6        | 0.11          |
| (1,2795) | 1:89:A:PHE:HB2   | 1:90:A:LYS:HA   | 16       | 0.11          |
| (1,2494) | 1:112:A:ILE:HD11 | 1:461:A:LYS:HE2 | 4        | 0.11          |
| (1,2494) | 1:112:A:ILE:HD11 | 1:461:A:LYS:HE3 | 4        | 0.11          |
| (1,2494) | 1:112:A:ILE:HD12 | 1:461:A:LYS:HE2 | 4        | 0.11          |
| (1,2494) | 1:112:A:ILE:HD12 | 1:461:A:LYS:HE3 | 4        | 0.11          |
| (1,2494) | 1:112:A:ILE:HD13 | 1:461:A:LYS:HE2 | 4        | 0.11          |
| (1,2494) | 1:112:A:ILE:HD13 | 1:461:A:LYS:HE3 | 4        | 0.11          |
| (1,2456) | 1:47:A:GLU:HA    | 1:50:A:ASP:HB2  | 3        | 0.11          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB2  | 9        | 0.11          |
| (1,2378) | 1:83:A:GLN:HG2   | 1:86:A:LEU:HB3  | 9        | 0.11          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB2  | 9        | 0.11          |
| (1,2378) | 1:83:A:GLN:HG3   | 1:86:A:LEU:HB3  | 9        | 0.11          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD11 | 20       | 0.11          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD12 | 20       | 0.11          |
| (1,2184) | 1:85:A:LEU:HA    | 1:85:A:LEU:HD13 | 20       | 0.11          |
| (1,2100) | 1:76:A:LEU:HD11  | 1:80:A:ASP:HB2  | 9        | 0.11          |
| (1,2100) | 1:76:A:LEU:HD11  | 1:80:A:ASP:HB3  | 9        | 0.11          |
| (1,2100) | 1:76:A:LEU:HD12  | 1:80:A:ASP:HB2  | 9        | 0.11          |
| (1,2100) | 1:76:A:LEU:HD12  | 1:80:A:ASP:HB3  | 9        | 0.11          |
| (1,2100) | 1:76:A:LEU:HD13  | 1:80:A:ASP:HB2  | 9        | 0.11          |
| (1,2100) | 1:76:A:LEU:HD13  | 1:80:A:ASP:HB3  | 9        | 0.11          |
| (1,1637) | 1:64:A:GLU:H     | 1:68:A:PHE:HA   | 19       | 0.11          |
| (1,1610) | 1:57:A:VAL:H     | 1:67:A:GLU:H    | 9        | 0.11          |
| (1,1610) | 1:57:A:VAL:H     | 1:67:A:GLU:H    | 14       | 0.11          |
| (1,1370) | 1:71:A:LEU:HB3   | 1:74:A:ARG:H    | 10       | 0.11          |
| (1,1177) | 1:470:A:ARG:HE   | 1:471:A:MET:HA  | 17       | 0.11          |
| (1,1081) | 1:144:A:LEU:HA   | 1:459:A:ARG:HE  | 1        | 0.11          |
| (1,1081) | 1:144:A:LEU:HA   | 1:459:A:ARG:HE  | 11       | 0.11          |
| (1,911)  | 1:89:A:PHE:H     | 1:140:A:PHE:HD1 | 18       | 0.11          |
| (1,911)  | 1:89:A:PHE:H     | 1:140:A:PHE:HD2 | 18       | 0.11          |
| (1,875)  | 1:69:A:LEU:H     | 1:71:A:LEU:HB2  | 8        | 0.11          |
| (1,875)  | 1:69:A:LEU:H     | 1:71:A:LEU:HB2  | 16       | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,817)  | 1:68:A:PHE:HB2  | 1:71:A:LEU:H     | 3        | 0.11          |
| (1,817)  | 1:68:A:PHE:HB2  | 1:71:A:LEU:H     | 7        | 0.11          |
| (1,802)  | 1:121:A:VAL:HB  | 1:123:A:ASP:H    | 7        | 0.11          |
| (1,802)  | 1:121:A:VAL:HB  | 1:123:A:ASP:H    | 10       | 0.11          |
| (1,799)  | 1:58:A:ASP:HB2  | 1:60:A:ASN:H     | 16       | 0.11          |
| (1,513)  | 1:80:A:ASP:H    | 1:81:A:SER:H     | 9        | 0.11          |
| (1,471)  | 1:91:A:VAL:HG21 | 1:93:A:ASP:H     | 10       | 0.11          |
| (1,471)  | 1:91:A:VAL:HG22 | 1:93:A:ASP:H     | 10       | 0.11          |
| (1,471)  | 1:91:A:VAL:HG23 | 1:93:A:ASP:H     | 10       | 0.11          |
| (1,451)  | 1:473:A:SER:HA  | 1:474:A:VAL:H    | 2        | 0.11          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB1  | 9        | 0.11          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB2  | 9        | 0.11          |
| (1,370)  | 1:129:A:SER:H   | 1:142:A:ALA:HB3  | 9        | 0.11          |
| (1,369)  | 1:126:A:ARG:HG3 | 1:129:A:SER:H    | 8        | 0.11          |
| (1,289)  | 1:135:A:ILE:H   | 1:139:A:GLN:HB3  | 8        | 0.11          |
| (1,289)  | 1:135:A:ILE:H   | 1:139:A:GLN:HB3  | 15       | 0.11          |
| (1,166)  | 1:66:A:SER:H    | 1:69:A:LEU:HG    | 13       | 0.11          |
| (1,162)  | 1:112:A:ILE:H   | 1:113:A:GLY:HA3  | 11       | 0.11          |
| (1,129)  | 1:98:A:GLY:H    | 1:99:A:LEU:HB2   | 3        | 0.11          |
| (1,129)  | 1:98:A:GLY:H    | 1:99:A:LEU:HB2   | 8        | 0.11          |
| (1,60)   | 1:94:A:LYS:HG2  | 1:96:A:GLY:H     | 15       | 0.11          |
| (1,60)   | 1:94:A:LYS:HG3  | 1:96:A:GLY:H     | 15       | 0.11          |
| (1,3541) | 1:92:A:PHE:HB2  | 1:105:A:LEU:HD11 | 9        | 0.1           |
| (1,3541) | 1:92:A:PHE:HB2  | 1:105:A:LEU:HD12 | 9        | 0.1           |
| (1,3541) | 1:92:A:PHE:HB2  | 1:105:A:LEU:HD13 | 9        | 0.1           |
| (1,3541) | 1:92:A:PHE:HB2  | 1:105:A:LEU:HD21 | 9        | 0.1           |
| (1,3541) | 1:92:A:PHE:HB2  | 1:105:A:LEU:HD22 | 9        | 0.1           |
| (1,3541) | 1:92:A:PHE:HB2  | 1:105:A:LEU:HD23 | 9        | 0.1           |
| (1,2933) | 1:473:A:SER:HB2 | 1:474:A:VAL:HB   | 20       | 0.1           |
| (1,2933) | 1:473:A:SER:HB3 | 1:474:A:VAL:HB   | 20       | 0.1           |
| (1,2378) | 1:83:A:GLN:HG2  | 1:86:A:LEU:HB2   | 3        | 0.1           |
| (1,2378) | 1:83:A:GLN:HG2  | 1:86:A:LEU:HB3   | 3        | 0.1           |
| (1,2378) | 1:83:A:GLN:HG3  | 1:86:A:LEU:HB2   | 3        | 0.1           |
| (1,2378) | 1:83:A:GLN:HG3  | 1:86:A:LEU:HB3   | 3        | 0.1           |
| (1,2197) | 1:9:A:ILE:HG21  | 1:69:A:LEU:HD11  | 16       | 0.1           |
| (1,2197) | 1:9:A:ILE:HG21  | 1:69:A:LEU:HD12  | 16       | 0.1           |
| (1,2197) | 1:9:A:ILE:HG21  | 1:69:A:LEU:HD13  | 16       | 0.1           |
| (1,2197) | 1:9:A:ILE:HG22  | 1:69:A:LEU:HD11  | 16       | 0.1           |
| (1,2197) | 1:9:A:ILE:HG22  | 1:69:A:LEU:HD12  | 16       | 0.1           |
| (1,2197) | 1:9:A:ILE:HG22  | 1:69:A:LEU:HD13  | 16       | 0.1           |
| (1,2197) | 1:9:A:ILE:HG23  | 1:69:A:LEU:HD11  | 16       | 0.1           |
| (1,2197) | 1:9:A:ILE:HG23  | 1:69:A:LEU:HD12  | 16       | 0.1           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2197) | 1:9:A:ILE:HG23  | 1:69:A:LEU:HD13  | 16       | 0.1           |
| (1,2062) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD11 | 20       | 0.1           |
| (1,2062) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD12 | 20       | 0.1           |
| (1,2062) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD13 | 20       | 0.1           |
| (1,1637) | 1:64:A:GLU:H    | 1:68:A:PHE:HA    | 18       | 0.1           |
| (1,1629) | 1:63:A:ILE:HG13 | 1:64:A:GLU:H     | 12       | 0.1           |
| (1,1600) | 1:55:A:ILE:HB   | 1:57:A:VAL:H     | 12       | 0.1           |
| (1,1297) | 1:67:A:GLU:HG3  | 1:70:A:ALA:H     | 13       | 0.1           |
| (1,1297) | 1:67:A:GLU:HG3  | 1:70:A:ALA:H     | 17       | 0.1           |
| (1,911)  | 1:89:A:PHE:H    | 1:140:A:PHE:HD1  | 8        | 0.1           |
| (1,911)  | 1:89:A:PHE:H    | 1:140:A:PHE:HD2  | 8        | 0.1           |
| (1,849)  | 1:83:A:GLN:HG2  | 1:86:A:LEU:H     | 9        | 0.1           |
| (1,849)  | 1:83:A:GLN:HG3  | 1:86:A:LEU:H     | 9        | 0.1           |
| (1,513)  | 1:80:A:ASP:H    | 1:81:A:SER:H     | 3        | 0.1           |
| (1,461)  | 1:131:A:GLY:HA3 | 1:132:A:SER:H    | 4        | 0.1           |
| (1,289)  | 1:135:A:ILE:H   | 1:139:A:GLN:HB3  | 2        | 0.1           |
| (1,162)  | 1:112:A:ILE:H   | 1:113:A:GLY:HA3  | 17       | 0.1           |
| (1,129)  | 1:98:A:GLY:H    | 1:99:A:LEU:HB2   | 12       | 0.1           |
| (1,129)  | 1:98:A:GLY:H    | 1:99:A:LEU:HB2   | 16       | 0.1           |
| (1,129)  | 1:98:A:GLY:H    | 1:99:A:LEU:HB2   | 18       | 0.1           |
| (1,117)  | 1:16:A:PHE:H    | 1:19:A:PHE:H     | 16       | 0.1           |
| (1,60)   | 1:94:A:LYS:HG2  | 1:96:A:GLY:H     | 10       | 0.1           |
| (1,60)   | 1:94:A:LYS:HG3  | 1:96:A:GLY:H     | 10       | 0.1           |

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

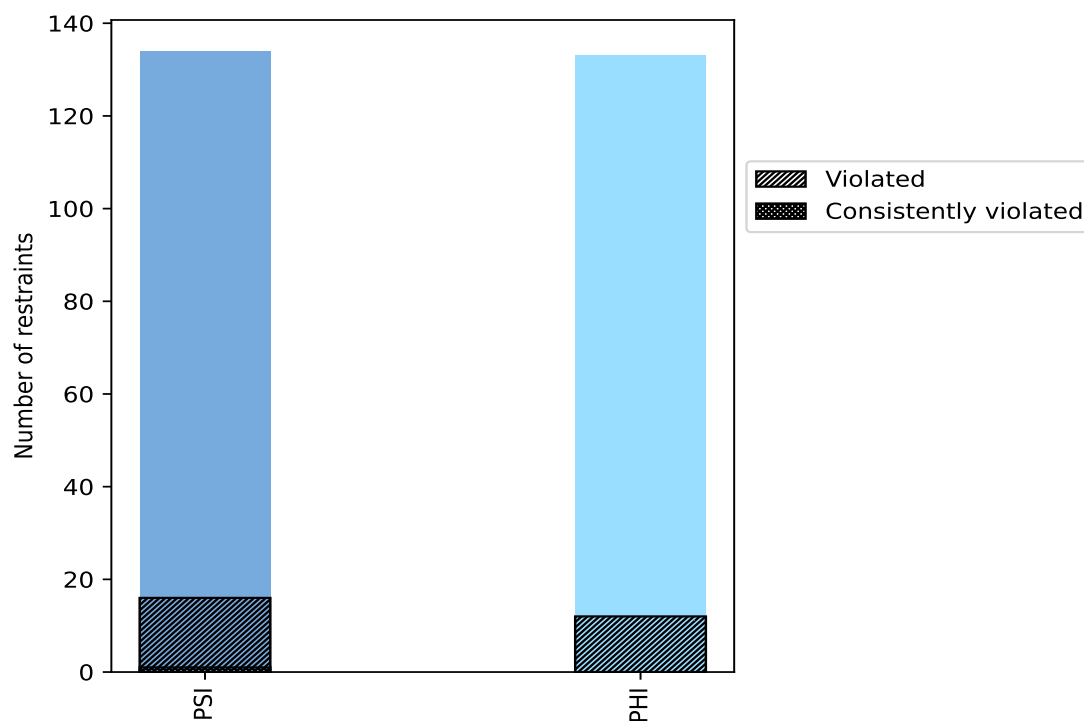
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 134   | 50.2           | 16                    | 11.9           | 6.0            | 1                                  | 0.7            | 0.4            |
| PHI        | 133   | 49.8           | 12                    | 9.0            | 4.5            | 0                                  | 0.0            | 0.0            |
| Total      | 267   | 100.0          | 28                    | 10.5           | 10.5           | 1                                  | 0.4            | 0.4            |

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

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



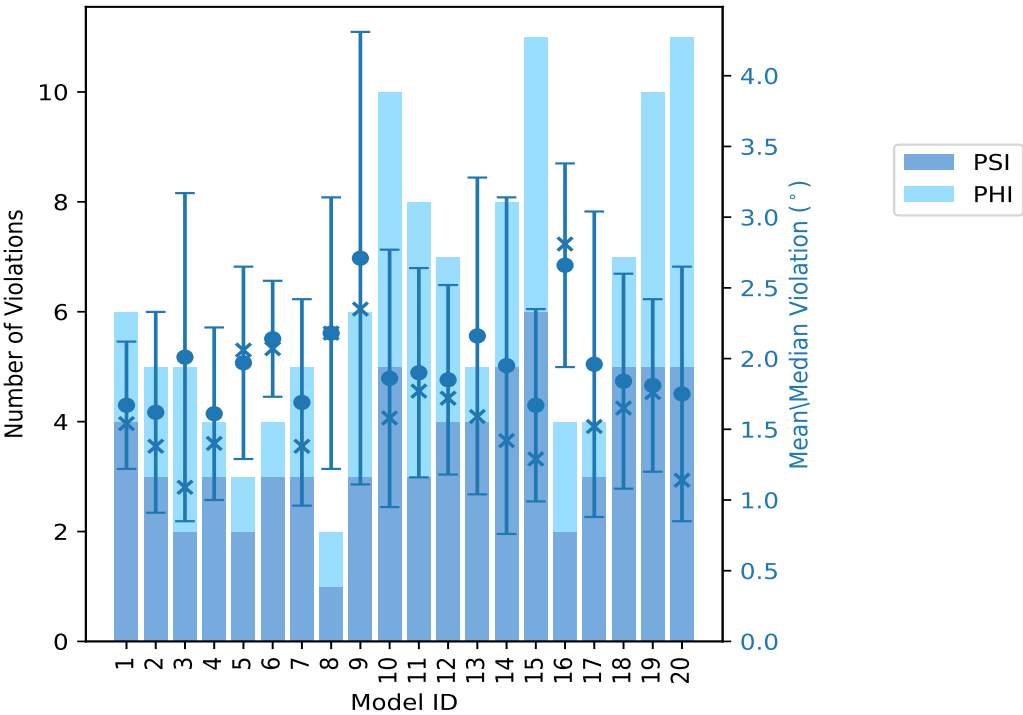
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 4                    | 2   | 6     | 1.67     | 2.5     | 0.45   | 1.54       |
| 2        | 3                    | 2   | 5     | 1.62     | 3.0     | 0.71   | 1.38       |
| 3        | 2                    | 3   | 5     | 2.01     | 3.56    | 1.16   | 1.09       |
| 4        | 3                    | 1   | 4     | 1.61     | 2.58    | 0.61   | 1.4        |
| 5        | 2                    | 1   | 3     | 1.97     | 2.76    | 0.68   | 2.06       |
| 6        | 3                    | 1   | 4     | 2.14     | 2.75    | 0.41   | 2.07       |
| 7        | 3                    | 2   | 5     | 1.69     | 3.08    | 0.73   | 1.38       |
| 8        | 1                    | 1   | 2     | 2.18     | 3.14    | 0.96   | 2.18       |
| 9        | 3                    | 3   | 6     | 2.71     | 5.13    | 1.6    | 2.35       |
| 10       | 5                    | 5   | 10    | 1.86     | 4.17    | 0.91   | 1.58       |
| 11       | 3                    | 5   | 8     | 1.9      | 3.56    | 0.74   | 1.77       |
| 12       | 4                    | 3   | 7     | 1.85     | 2.93    | 0.67   | 1.72       |
| 13       | 4                    | 1   | 5     | 2.16     | 3.76    | 1.12   | 1.59       |
| 14       | 5                    | 3   | 8     | 1.95     | 4.21    | 1.19   | 1.42       |
| 15       | 6                    | 5   | 11    | 1.67     | 2.8     | 0.68   | 1.29       |
| 16       | 2                    | 2   | 4     | 2.66     | 3.46    | 0.72   | 2.81       |
| 17       | 3                    | 1   | 4     | 1.96     | 3.79    | 1.08   | 1.52       |
| 18       | 5                    | 2   | 7     | 1.84     | 3.32    | 0.76   | 1.65       |
| 19       | 5                    | 5   | 10    | 1.81     | 2.73    | 0.61   | 1.76       |
| 20       | 5                    | 6   | 11    | 1.75     | 3.53    | 0.9    | 1.14       |

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



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

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

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

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

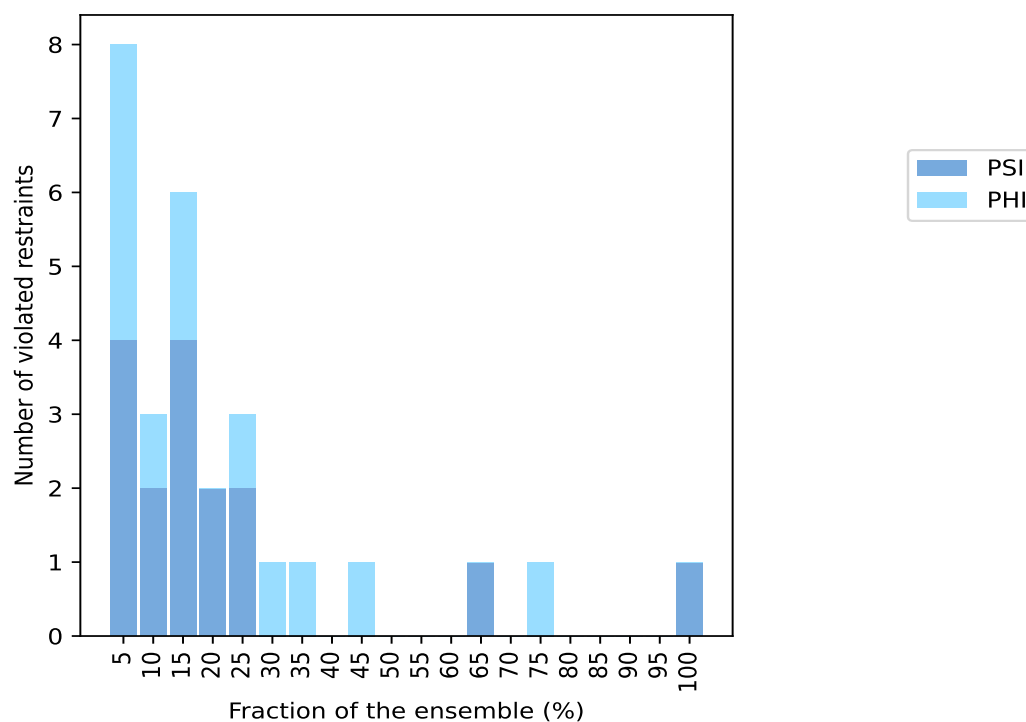
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |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

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

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

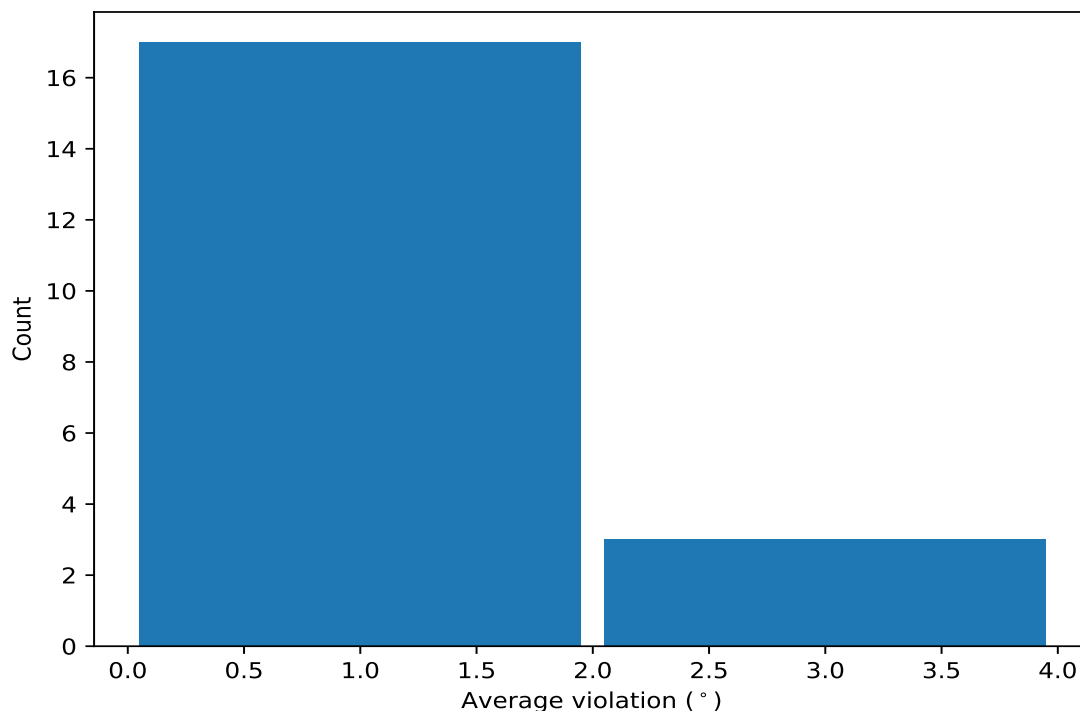


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 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.

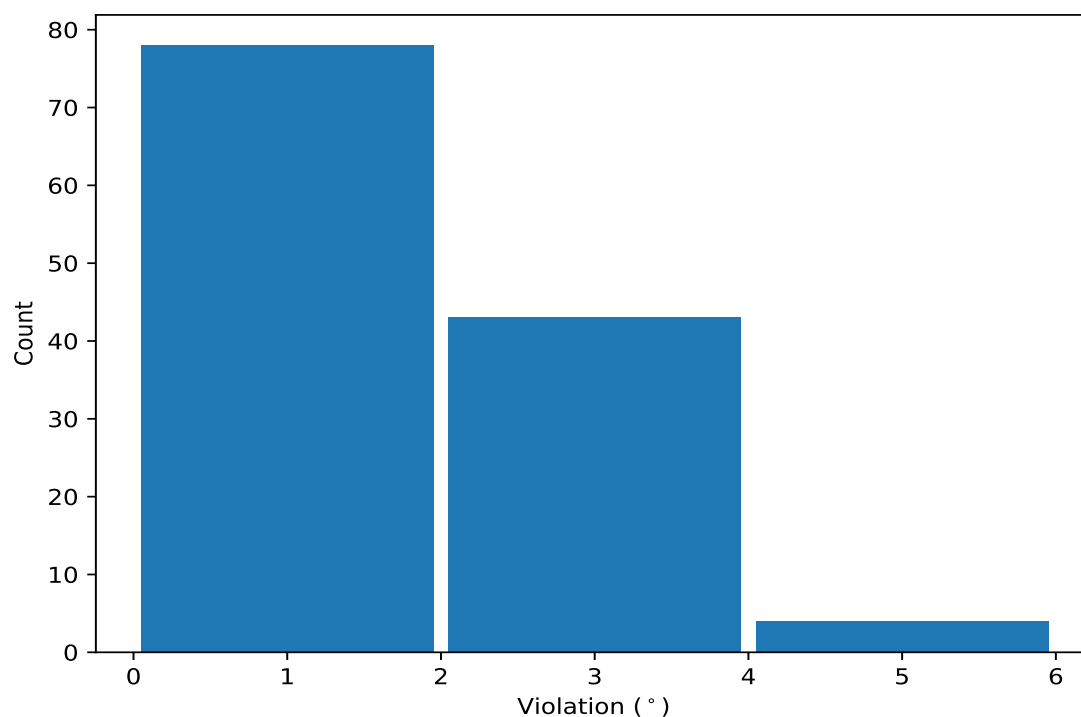
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C  | 1:106:A:LYS:N | 20                  | 3.25 | 0.52            | 3.23   |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 15                  | 1.68 | 0.42            | 1.66   |
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 13                  | 1.97 | 0.86            | 1.56   |
| (1,122) | 1:81:A:SER:C  | 1:82:A:GLU:N   | 1:82:A:GLU:CA  | 1:82:A:GLU:C  | 9                   | 2.65 | 1.04            | 2.47   |
| (1,194) | 1:122:A:ASP:C | 1:123:A:ASP:N  | 1:123:A:ASP:CA | 1:123:A:ASP:C | 7                   | 1.19 | 0.18            | 1.08   |
| (1,120) | 1:80:A:ASP:C  | 1:81:A:SER:N   | 1:81:A:SER:CA  | 1:81:A:SER:C  | 6                   | 1.85 | 0.66            | 1.72   |
| (1,92)  | 1:56:A:ASP:C  | 1:57:A:VAL:N   | 1:57:A:VAL:CA  | 1:57:A:VAL:C  | 5                   | 1.88 | 0.59            | 2.0    |
| (1,159) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C  | 1:104:A:GLU:N | 5                   | 1.49 | 0.22            | 1.53   |
| (1,115) | 1:70:A:ALA:N  | 1:70:A:ALA:CA  | 1:70:A:ALA:C   | 1:71:A:LEU:N  | 5                   | 1.28 | 0.38            | 1.12   |
| (1,129) | 1:85:A:LEU:N  | 1:85:A:LEU:CA  | 1:85:A:LEU:C   | 1:86:A:LEU:N  | 4                   | 1.7  | 0.41            | 1.72   |
| (1,157) | 1:102:A:ALA:N | 1:102:A:ALA:CA | 1:102:A:ALA:C  | 1:103:A:ALA:N | 4                   | 1.44 | 0.29            | 1.4    |
| (1,135) | 1:88:A:ALA:N  | 1:88:A:ALA:CA  | 1:88:A:ALA:C   | 1:89:A:PHE:N  | 3                   | 2.64 | 1.25            | 2.58   |
| (1,125) | 1:83:A:GLN:N  | 1:83:A:GLN:CA  | 1:83:A:GLN:C   | 1:84:A:GLU:N  | 3                   | 1.46 | 0.26            | 1.55   |
| (1,179) | 1:114:A:GLU:N | 1:114:A:GLU:CA | 1:114:A:GLU:C  | 1:115:A:LYS:N | 3                   | 1.25 | 0.19            | 1.15   |
| (1,134) | 1:87:A:GLU:C  | 1:88:A:ALA:N   | 1:88:A:ALA:CA  | 1:88:A:ALA:C  | 3                   | 1.2  | 0.07            | 1.19   |
| (1,254) | 1:467:A:LYS:C | 1:468:A:VAL:N  | 1:468:A:VAL:CA | 1:468:A:VAL:C | 3                   | 1.12 | 0.04            | 1.11   |
| (1,251) | 1:466:A:ALA:N | 1:466:A:ALA:CA | 1:466:A:ALA:C  | 1:467:A:LYS:N | 3                   | 1.11 | 0.02            | 1.12   |
| (1,38)  | 1:26:A:SER:N  | 1:26:A:SER:CA  | 1:26:A:SER:C   | 1:27:A:ILE:N  | 2                   | 1.26 | 0.25            | 1.26   |
| (1,76)  | 1:47:A:GLU:C  | 1:48:A:VAL:N   | 1:48:A:VAL:CA  | 1:48:A:VAL:C  | 2                   | 1.18 | 0.09            | 1.18   |
| (1,69)  | 1:44:A:SER:N  | 1:44:A:SER:CA  | 1:44:A:SER:C   | 1:45:A:GLU:N  | 2                   | 1.04 | 0.03            | 1.04   |

<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 (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,122) | 1:81:A:SER:C  | 1:82:A:GLU:N   | 1:82:A:GLU:CA | 1:82:A:GLU:C  | 9        | 5.13          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C | 1:106:A:LYS:N | 9        | 4.21          |
| (1,135) | 1:88:A:ALA:N  | 1:88:A:ALA:CA  | 1:88:A:ALA:C  | 1:89:A:PHE:N  | 14       | 4.21          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C | 1:106:A:LYS:N | 10       | 4.17          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C | 1:106:A:LYS:N | 17       | 3.79          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C | 1:106:A:LYS:N | 13       | 3.76          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C | 1:106:A:LYS:N | 14       | 3.74          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C | 1:106:A:LYS:N | 3        | 3.56          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C | 1:106:A:LYS:N | 11       | 3.56          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C | 1:106:A:LYS:N | 20       | 3.53          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C | 1:106:A:LYS:N | 16       | 3.46          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 9        | 3.33          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C  | 1:106:A:LYS:N | 18       | 3.32          |
| (1,122) | 1:81:A:SER:C  | 1:82:A:GLU:N   | 1:82:A:GLU:CA  | 1:82:A:GLU:C  | 3        | 3.3           |
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 13       | 3.24          |
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 20       | 3.16          |
| (1,120) | 1:80:A:ASP:C  | 1:81:A:SER:N   | 1:81:A:SER:CA  | 1:81:A:SER:C  | 16       | 3.15          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C  | 1:106:A:LYS:N | 8        | 3.14          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C  | 1:106:A:LYS:N | 7        | 3.08          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C  | 1:106:A:LYS:N | 2        | 3.0           |
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 12       | 2.93          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C  | 1:106:A:LYS:N | 15       | 2.8           |
| (1,92)  | 1:56:A:ASP:C  | 1:57:A:VAL:N   | 1:57:A:VAL:CA  | 1:57:A:VAL:C  | 20       | 2.78          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C  | 1:106:A:LYS:N | 5        | 2.76          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C  | 1:106:A:LYS:N | 6        | 2.75          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C  | 1:106:A:LYS:N | 19       | 2.73          |
| (1,122) | 1:81:A:SER:C  | 1:82:A:GLU:N   | 1:82:A:GLU:CA  | 1:82:A:GLU:C  | 19       | 2.66          |
| (1,122) | 1:81:A:SER:C  | 1:82:A:GLU:N   | 1:82:A:GLU:CA  | 1:82:A:GLU:C  | 15       | 2.65          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C  | 1:106:A:LYS:N | 12       | 2.63          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C  | 1:106:A:LYS:N | 4        | 2.58          |
| (1,135) | 1:88:A:ALA:N  | 1:88:A:ALA:CA  | 1:88:A:ALA:C   | 1:89:A:PHE:N  | 15       | 2.58          |
| (1,163) | 1:105:A:LEU:N | 1:105:A:LEU:CA | 1:105:A:LEU:C  | 1:106:A:LYS:N | 1        | 2.5           |
| (1,122) | 1:81:A:SER:C  | 1:82:A:GLU:N   | 1:82:A:GLU:CA  | 1:82:A:GLU:C  | 16       | 2.47          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 19       | 2.37          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 18       | 2.36          |
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 10       | 2.33          |
| (1,122) | 1:81:A:SER:C  | 1:82:A:GLU:N   | 1:82:A:GLU:CA  | 1:82:A:GLU:C  | 10       | 2.32          |
| (1,122) | 1:81:A:SER:C  | 1:82:A:GLU:N   | 1:82:A:GLU:CA  | 1:82:A:GLU:C  | 11       | 2.28          |
| (1,129) | 1:85:A:LEU:N  | 1:85:A:LEU:CA  | 1:85:A:LEU:C   | 1:86:A:LEU:N  | 6        | 2.25          |
| (1,173) | 1:110:A:THR:N | 1:110:A:THR:CA | 1:110:A:THR:C  | 1:111:A:SER:N | 10       | 2.16          |
| (1,92)  | 1:56:A:ASP:C  | 1:57:A:VAL:N   | 1:57:A:VAL:CA  | 1:57:A:VAL:C  | 18       | 2.13          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 12       | 2.07          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 5        | 2.06          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 15       | 2.04          |
| (1,115) | 1:70:A:ALA:N  | 1:70:A:ALA:CA  | 1:70:A:ALA:C   | 1:71:A:LEU:N  | 11       | 2.04          |
| (1,120) | 1:80:A:ASP:C  | 1:81:A:SER:N   | 1:81:A:SER:CA  | 1:81:A:SER:C  | 19       | 2.01          |
| (1,92)  | 1:56:A:ASP:C  | 1:57:A:VAL:N   | 1:57:A:VAL:CA  | 1:57:A:VAL:C  | 19       | 2.0           |
| (1,120) | 1:80:A:ASP:C  | 1:81:A:SER:N   | 1:81:A:SER:CA  | 1:81:A:SER:C  | 11       | 1.99          |
| (1,122) | 1:81:A:SER:C  | 1:82:A:GLU:N   | 1:82:A:GLU:CA  | 1:82:A:GLU:C  | 1        | 1.91          |
| (1,157) | 1:102:A:ALA:N | 1:102:A:ALA:CA | 1:102:A:ALA:C  | 1:103:A:ALA:N | 6        | 1.89          |
| (1,129) | 1:85:A:LEU:N  | 1:85:A:LEU:CA  | 1:85:A:LEU:C   | 1:86:A:LEU:N  | 20       | 1.82          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 7        | 1.74          |
| (1,159) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C  | 1:104:A:GLU:N | 12       | 1.72          |
| (1,125) | 1:83:A:GLN:N  | 1:83:A:GLN:CA  | 1:83:A:GLN:C   | 1:84:A:GLU:N  | 10       | 1.72          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 4        | 1.68          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 6        | 1.66          |
| (1,159) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C  | 1:104:A:GLU:N | 18       | 1.65          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 17       | 1.62          |
| (1,129) | 1:85:A:LEU:N  | 1:85:A:LEU:CA  | 1:85:A:LEU:C   | 1:86:A:LEU:N  | 1        | 1.61          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 13       | 1.59          |
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 16       | 1.58          |
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 14       | 1.56          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 11       | 1.55          |
| (1,125) | 1:83:A:GLN:N  | 1:83:A:GLN:CA  | 1:83:A:GLN:C   | 1:84:A:GLU:N  | 15       | 1.55          |
| (1,194) | 1:122:A:ASP:C | 1:123:A:ASP:N  | 1:123:A:ASP:CA | 1:123:A:ASP:C | 11       | 1.53          |
| (1,159) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C  | 1:104:A:GLU:N | 19       | 1.53          |
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 2        | 1.53          |
| (1,179) | 1:114:A:GLU:N | 1:114:A:GLU:CA | 1:114:A:GLU:C  | 1:115:A:LYS:N | 19       | 1.52          |
| (1,38)  | 1:26:A:SER:N  | 1:26:A:SER:CA  | 1:26:A:SER:C   | 1:27:A:ILE:N  | 14       | 1.51          |
| (1,159) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C  | 1:104:A:GLU:N | 1        | 1.46          |
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 1        | 1.46          |
| (1,120) | 1:80:A:ASP:C  | 1:81:A:SER:N   | 1:81:A:SER:CA  | 1:81:A:SER:C  | 10       | 1.45          |
| (1,157) | 1:102:A:ALA:N | 1:102:A:ALA:CA | 1:102:A:ALA:C  | 1:103:A:ALA:N | 17       | 1.42          |
| (1,258) | 1:469:A:SER:C | 1:470:A:ARG:N  | 1:470:A:ARG:CA | 1:470:A:ARG:C | 2        | 1.38          |
| (1,157) | 1:102:A:ALA:N | 1:102:A:ALA:CA | 1:102:A:ALA:C  | 1:103:A:ALA:N | 7        | 1.38          |
| (1,120) | 1:80:A:ASP:C  | 1:81:A:SER:N   | 1:81:A:SER:CA  | 1:81:A:SER:C  | 9        | 1.36          |
| (1,194) | 1:122:A:ASP:C | 1:123:A:ASP:N  | 1:123:A:ASP:CA | 1:123:A:ASP:C | 20       | 1.34          |
| (1,92)  | 1:56:A:ASP:C  | 1:57:A:VAL:N   | 1:57:A:VAL:CA  | 1:57:A:VAL:C  | 14       | 1.32          |
| (1,134) | 1:87:A:GLU:C  | 1:88:A:ALA:N   | 1:88:A:ALA:CA  | 1:88:A:ALA:C  | 15       | 1.29          |
| (1,194) | 1:122:A:ASP:C | 1:123:A:ASP:N  | 1:123:A:ASP:CA | 1:123:A:ASP:C | 12       | 1.28          |
| (1,76)  | 1:47:A:GLU:C  | 1:48:A:VAL:N   | 1:48:A:VAL:CA  | 1:48:A:VAL:C  | 12       | 1.28          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 8        | 1.22          |
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 15       | 1.21          |
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 18       | 1.21          |
| (1,242) | 1:461:A:LYS:C | 1:462:A:ILE:N  | 1:462:A:ILE:CA | 1:462:A:ILE:C | 19       | 1.2           |
| (1,134) | 1:87:A:GLU:C  | 1:88:A:ALA:N   | 1:88:A:ALA:CA  | 1:88:A:ALA:C  | 10       | 1.19          |
| (1,254) | 1:467:A:LYS:C | 1:468:A:VAL:N  | 1:468:A:VAL:CA | 1:468:A:VAL:C | 11       | 1.17          |
| (1,120) | 1:80:A:ASP:C  | 1:81:A:SER:N   | 1:81:A:SER:CA  | 1:81:A:SER:C  | 2        | 1.16          |
| (1,92)  | 1:56:A:ASP:C  | 1:57:A:VAL:N   | 1:57:A:VAL:CA  | 1:57:A:VAL:C  | 10       | 1.16          |
| (1,179) | 1:114:A:GLU:N | 1:114:A:GLU:CA | 1:114:A:GLU:C  | 1:115:A:LYS:N | 7        | 1.15          |
| (1,251) | 1:466:A:ALA:N | 1:466:A:ALA:CA | 1:466:A:ALA:C  | 1:467:A:LYS:N | 15       | 1.14          |
| (1,135) | 1:88:A:ALA:N  | 1:88:A:ALA:CA  | 1:88:A:ALA:C   | 1:89:A:PHE:N  | 20       | 1.14          |
| (1,121) | 1:81:A:SER:N  | 1:81:A:SER:CA  | 1:81:A:SER:C   | 1:82:A:GLU:N  | 20       | 1.13          |
| (1,251) | 1:466:A:ALA:N | 1:466:A:ALA:CA | 1:466:A:ALA:C  | 1:467:A:LYS:N | 18       | 1.12          |
| (1,122) | 1:81:A:SER:C  | 1:82:A:GLU:N   | 1:82:A:GLU:CA  | 1:82:A:GLU:C  | 20       | 1.12          |
| (1,115) | 1:70:A:ALA:N  | 1:70:A:ALA:CA  | 1:70:A:ALA:C   | 1:71:A:LEU:N  | 9        | 1.12          |
| (1,115) | 1:70:A:ALA:N  | 1:70:A:ALA:CA  | 1:70:A:ALA:C   | 1:71:A:LEU:N  | 13       | 1.12          |
| (1,254) | 1:467:A:LYS:C | 1:468:A:VAL:N  | 1:468:A:VAL:CA | 1:468:A:VAL:C | 9        | 1.11          |
| (1,134) | 1:87:A:GLU:C  | 1:88:A:ALA:N   | 1:88:A:ALA:CA  | 1:88:A:ALA:C  | 14       | 1.11          |
| (1,129) | 1:85:A:LEU:N  | 1:85:A:LEU:CA  | 1:85:A:LEU:C   | 1:86:A:LEU:N  | 4        | 1.11          |
| (1,125) | 1:83:A:GLN:N  | 1:83:A:GLN:CA  | 1:83:A:GLN:C   | 1:84:A:GLU:N  | 18       | 1.1           |
| (1,179) | 1:114:A:GLU:N | 1:114:A:GLU:CA | 1:114:A:GLU:C  | 1:115:A:LYS:N | 5        | 1.09          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 3        | 1.09          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 14       | 1.09          |
| (1,159) | 1:103:A:ALA:N | 1:103:A:ALA:CA | 1:103:A:ALA:C  | 1:104:A:GLU:N | 14       | 1.09          |
| (1,157) | 1:102:A:ALA:N | 1:102:A:ALA:CA | 1:102:A:ALA:C  | 1:103:A:ALA:N | 13       | 1.09          |
| (1,146) | 1:93:A:ASP:C  | 1:94:A:LYS:N   | 1:94:A:LYS:CA  | 1:94:A:LYS:C  | 20       | 1.09          |
| (1,76)  | 1:47:A:GLU:C  | 1:48:A:VAL:N   | 1:48:A:VAL:CA  | 1:48:A:VAL:C  | 3        | 1.09          |
| (1,254) | 1:467:A:LYS:C | 1:468:A:VAL:N  | 1:468:A:VAL:CA | 1:468:A:VAL:C | 20       | 1.08          |
| (1,251) | 1:466:A:ALA:N | 1:466:A:ALA:CA | 1:466:A:ALA:C  | 1:467:A:LYS:N | 4        | 1.08          |
| (1,194) | 1:122:A:ASP:C | 1:123:A:ASP:N  | 1:123:A:ASP:CA | 1:123:A:ASP:C | 7        | 1.08          |
| (1,194) | 1:122:A:ASP:C | 1:123:A:ASP:N  | 1:123:A:ASP:CA | 1:123:A:ASP:C | 1        | 1.07          |
| (1,69)  | 1:44:A:SER:N  | 1:44:A:SER:CA  | 1:44:A:SER:C   | 1:45:A:GLU:N  | 11       | 1.06          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,52)  | 1:33:A:ALA:N  | 1:33:A:ALA:CA  | 1:33:A:ALA:C   | 1:34:A:THR:N  | 15       | 1.06          |
| (1,177) | 1:112:A:ILE:N | 1:112:A:ILE:CA | 1:112:A:ILE:C  | 1:113:A:GLY:N | 19       | 1.05          |
| (1,160) | 1:103:A:ALA:C | 1:104:A:GLU:N  | 1:104:A:GLU:CA | 1:104:A:GLU:C | 20       | 1.05          |
| (1,115) | 1:70:A:ALA:N  | 1:70:A:ALA:CA  | 1:70:A:ALA:C   | 1:71:A:LEU:N  | 10       | 1.05          |
| (1,115) | 1:70:A:ALA:N  | 1:70:A:ALA:CA  | 1:70:A:ALA:C   | 1:71:A:LEU:N  | 12       | 1.05          |
| (1,260) | 1:470:A:ARG:C | 1:471:A:MET:N  | 1:471:A:MET:CA | 1:471:A:MET:C | 15       | 1.04          |
| (1,194) | 1:122:A:ASP:C | 1:123:A:ASP:N  | 1:123:A:ASP:CA | 1:123:A:ASP:C | 15       | 1.03          |
| (1,194) | 1:122:A:ASP:C | 1:123:A:ASP:N  | 1:123:A:ASP:CA | 1:123:A:ASP:C | 10       | 1.02          |
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 3        | 1.02          |
| (1,107) | 1:65:A:PHE:N  | 1:65:A:PHE:CA  | 1:65:A:PHE:C   | 1:66:A:SER:N  | 17       | 1.02          |
| (1,69)  | 1:44:A:SER:N  | 1:44:A:SER:CA  | 1:44:A:SER:C   | 1:45:A:GLU:N  | 2        | 1.01          |
| (1,38)  | 1:26:A:SER:N  | 1:26:A:SER:CA  | 1:26:A:SER:C   | 1:27:A:ILE:N  | 19       | 1.01          |