



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 02:25 PM EST

PDB ID : 2L4N  
BMRB ID : 17245  
Title : Solution Structure of the Chemokine CCL21  
Authors : Veldkamp, C.T.; Peterson, F.C.; Love, M.; Sandberg, J.L.  
Deposited on : 2010-10-10

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)

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<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 : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.40

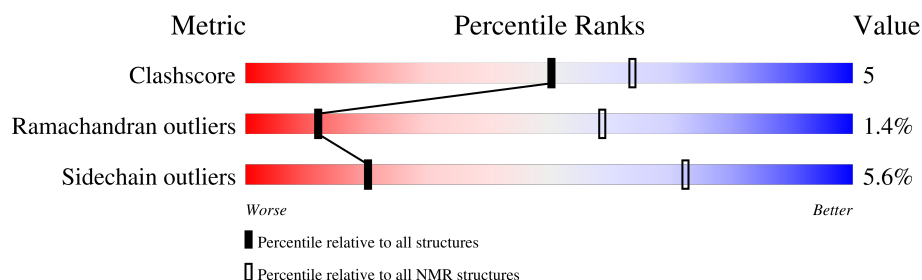
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 84%.

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



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 210492                      | 14027                     |
| Ramachandran outliers | 207382                      | 12486                     |
| Sidechain outliers    | 206894                      | 12463                     |

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     | 113    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:8-A:70 (63)         | 1.03              | 19           |

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

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

The models can be grouped into 4 clusters and 6 single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 1127 atoms, of which 572 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called C-C motif chemokine 21.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 70       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1127  | 348 | 572 | 102 | 100 | 5 |       |

There are 2 discrepancies between the modelled and reference sequences:

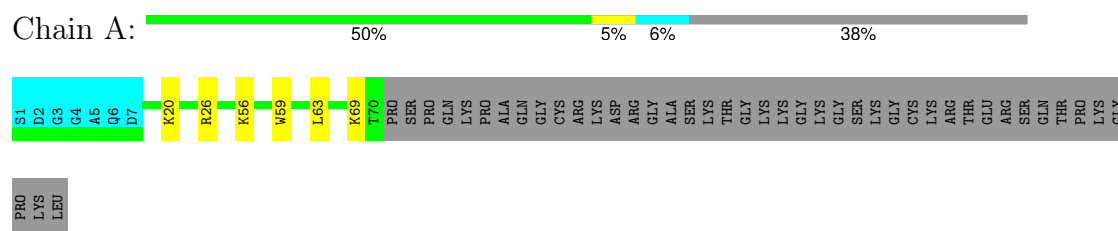
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 112     | LYS      | -      | expression tag | UNP O00585 |
| A     | 113     | LEU      | -      | expression tag | UNP O00585 |

## 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: C-C motif chemokine 21

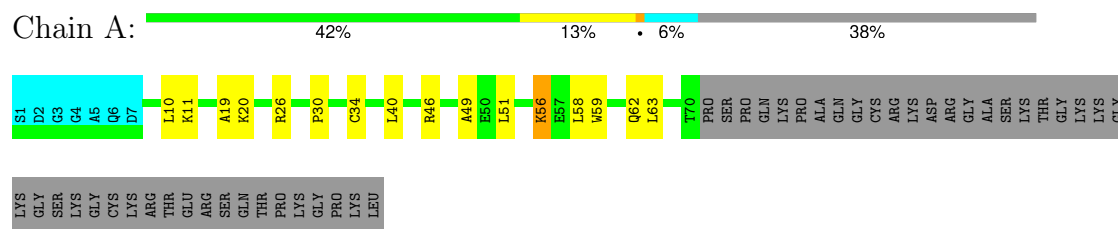


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

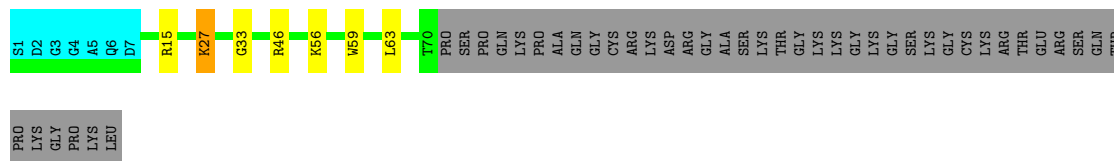
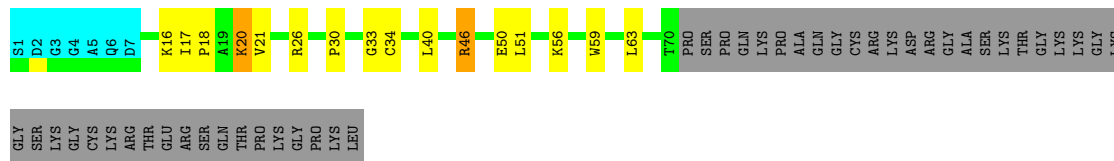
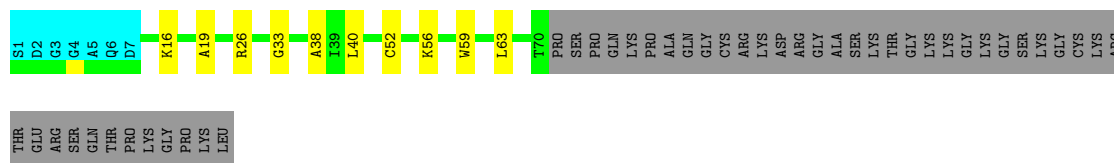
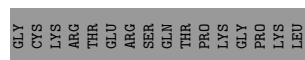
- Molecule 1: C-C motif chemokine 21

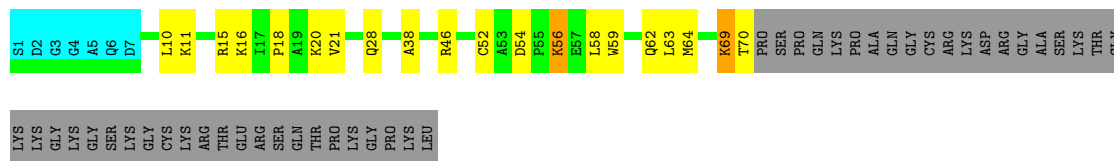
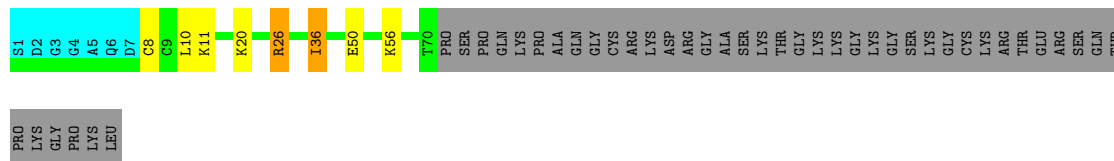
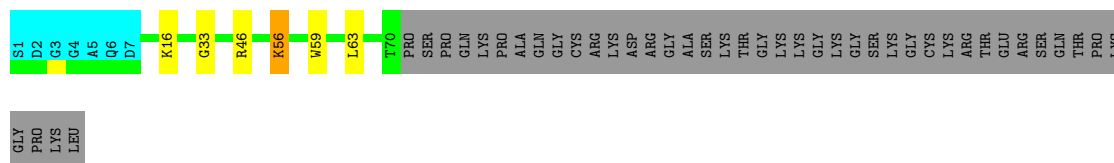
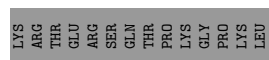


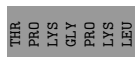
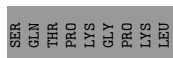
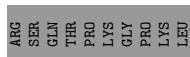
#### 4.2.2 Score per residue for model 2

- Molecule 1: C-C motif chemokine 21







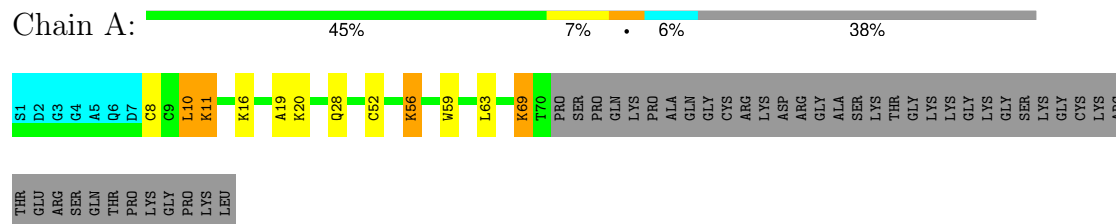






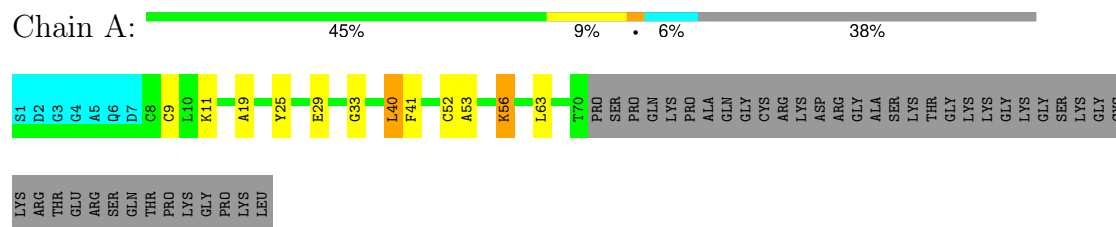
#### 4.2.15 Score per residue for model 15

- Molecule 1: C-C motif chemokine 21



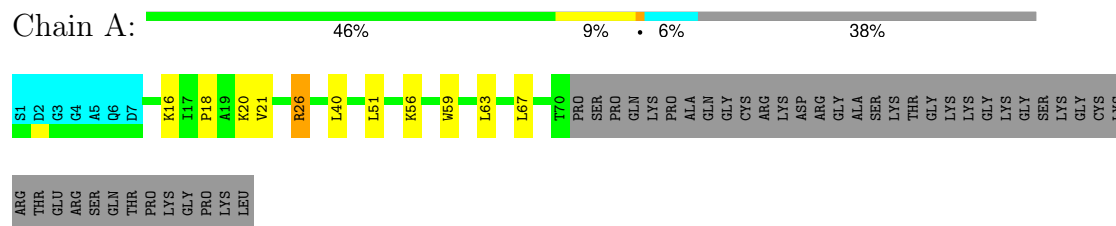
#### 4.2.16 Score per residue for model 16

- Molecule 1: C-C motif chemokine 21



#### 4.2.17 Score per residue for model 17

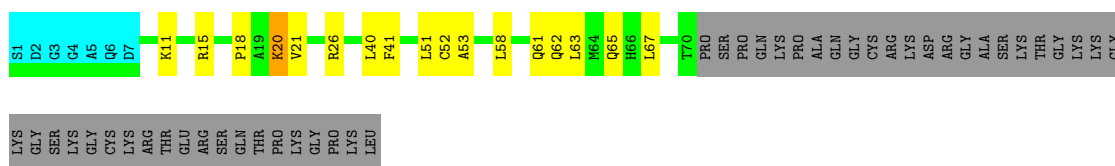
- Molecule 1: C-C motif chemokine 21



#### 4.2.18 Score per residue for model 18

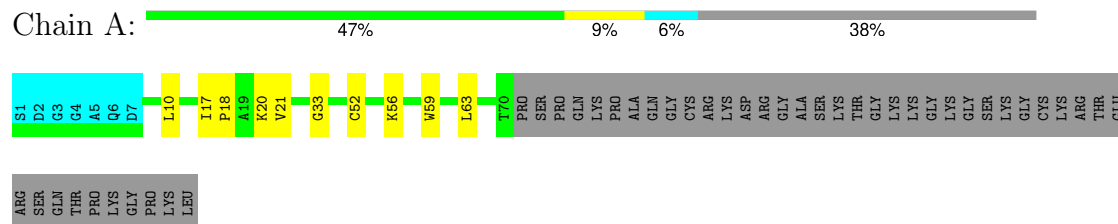
- Molecule 1: C-C motif chemokine 21





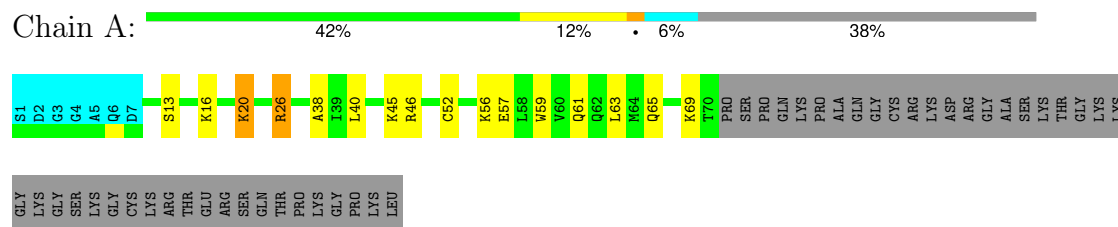
#### 4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: C-C motif chemokine 21



#### 4.2.20 Score per residue for model 20

- Molecule 1: C-C motif chemokine 21



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *AUTOMATED METHODS WERE USED FOR BACKBONE CHEMICAL SHIFT ASSIGNMENT AND ITERATIVE NOE REFINEMENT. FINAL STRUCTURES WERE OBTAINED BY MOLECULAR DYNAMICS IN EXPLICIT SOLVENT.*

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 |
|---------------|--------------------|---------|
| CYANA         | structure solution |         |
| CYANA         | refinement         |         |

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

|  |                |
|--|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1224           |
| Number of shifts mapped to atoms             | 811            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 413            |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 84%            |

## 6 Model quality [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 511   | 538      | 537      | 6±2     |
| All | All   | 10220 | 10760    | 10740    | 113     |

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 5.

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

| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:41:PHE:CE1 | 1:A:63:LEU:HD13 | 0.56     | 2.35        | 18     | 1     |
| 1:A:59:TRP:O   | 1:A:63:LEU:HG   | 0.56     | 2.00        | 20     | 15    |
| 1:A:41:PHE:CZ  | 1:A:63:LEU:HD13 | 0.56     | 2.36        | 18     | 1     |
| 1:A:69:LYS:N   | 1:A:69:LYS:HE2  | 0.55     | 2.17        | 13     | 1     |
| 1:A:11:LYS:O   | 1:A:52:CYS:HB3  | 0.54     | 2.02        | 16     | 3     |
| 1:A:46:ARG:HD3 | 1:A:46:ARG:O    | 0.53     | 2.03        | 10     | 3     |
| 1:A:69:LYS:HD2 | 1:A:70:THR:N    | 0.52     | 2.19        | 9      | 1     |
| 1:A:11:LYS:HD3 | 1:A:11:LYS:O    | 0.51     | 2.05        | 15     | 1     |
| 1:A:63:LEU:O   | 1:A:67:LEU:HG   | 0.51     | 2.06        | 2      | 5     |
| 1:A:69:LYS:N   | 1:A:69:LYS:HE3  | 0.51     | 2.21        | 11     | 3     |
| 1:A:26:ARG:HB3 | 1:A:40:LEU:HB2  | 0.49     | 1.84        | 6      | 5     |
| 1:A:38:ALA:HB1 | 1:A:52:CYS:SG   | 0.49     | 2.48        | 3      | 2     |
| 1:A:10:LEU:CD1 | 1:A:11:LYS:HG2  | 0.49     | 2.38        | 8      | 1     |
| 1:A:40:LEU:HA  | 1:A:51:LEU:O    | 0.48     | 2.09        | 18     | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:56:LYS:HE3  | 1:A:56:LYS:HA   | 0.48     | 1.86        | 7      | 1     |
| 1:A:10:LEU:HD23 | 1:A:52:CYS:SG   | 0.48     | 2.49        | 12     | 1     |
| 1:A:10:LEU:HD12 | 1:A:11:LYS:N    | 0.48     | 2.23        | 9      | 2     |
| 1:A:18:PRO:O    | 1:A:21:VAL:HG22 | 0.47     | 2.09        | 13     | 6     |
| 1:A:10:LEU:N    | 1:A:52:CYS:SG   | 0.47     | 2.86        | 6      | 3     |
| 1:A:10:LEU:H    | 1:A:10:LEU:HD23 | 0.47     | 1.68        | 15     | 1     |
| 1:A:65:GLN:O    | 1:A:69:LYS:HG3  | 0.47     | 2.09        | 20     | 1     |
| 1:A:66:HIS:O    | 1:A:69:LYS:HG2  | 0.46     | 2.10        | 2      | 1     |
| 1:A:20:LYS:HD2  | 1:A:20:LYS:H    | 0.46     | 1.70        | 13     | 6     |
| 1:A:25:TYR:HA   | 1:A:40:LEU:O    | 0.46     | 2.11        | 16     | 1     |
| 1:A:58:LEU:O    | 1:A:62:GLN:HG3  | 0.46     | 2.10        | 9      | 4     |
| 1:A:16:LYS:N    | 1:A:16:LYS:HD2  | 0.45     | 2.26        | 7      | 1     |
| 1:A:19:ALA:HB2  | 1:A:63:LEU:HD22 | 0.45     | 1.89        | 11     | 3     |
| 1:A:25:TYR:CE1  | 1:A:64:MET:HA   | 0.45     | 2.47        | 12     | 1     |
| 1:A:36:ILE:HD13 | 1:A:36:ILE:H    | 0.44     | 1.73        | 8      | 1     |
| 1:A:16:LYS:HD2  | 1:A:59:TRP:CZ2  | 0.44     | 2.47        | 11     | 1     |
| 1:A:56:LYS:HA   | 1:A:56:LYS:CE   | 0.43     | 2.43        | 7      | 1     |
| 1:A:8:CYS:HA    | 1:A:28:GLN:OE1  | 0.43     | 2.13        | 15     | 1     |
| 1:A:18:PRO:HG2  | 1:A:21:VAL:CG2  | 0.43     | 2.42        | 9      | 1     |
| 1:A:61:GLN:O    | 1:A:65:GLN:HG3  | 0.43     | 2.13        | 18     | 1     |
| 1:A:10:LEU:HD11 | 1:A:50:GLU:O    | 0.43     | 2.14        | 8      | 1     |
| 1:A:19:ALA:N    | 1:A:63:LEU:HD22 | 0.43     | 2.27        | 16     | 3     |
| 1:A:54:ASP:OD1  | 1:A:56:LYS:HB2  | 0.43     | 2.14        | 9      | 1     |
| 1:A:41:PHE:CE2  | 1:A:53:ALA:HB2  | 0.43     | 2.49        | 18     | 2     |
| 1:A:56:LYS:N    | 1:A:56:LYS:HD2  | 0.43     | 2.29        | 1      | 3     |
| 1:A:15:ARG:HA   | 1:A:15:ARG:NE   | 0.43     | 2.28        | 18     | 1     |
| 1:A:10:LEU:HD12 | 1:A:11:LYS:HG2  | 0.42     | 1.90        | 8      | 1     |
| 1:A:53:ALA:O    | 1:A:55:PRO:HD3  | 0.42     | 2.15        | 6      | 1     |
| 1:A:30:PRO:HA   | 1:A:34:CYS:O    | 0.42     | 2.15        | 1      | 1     |
| 1:A:26:ARG:HD3  | 1:A:26:ARG:C    | 0.42     | 2.34        | 10     | 2     |
| 1:A:57:GLU:O    | 1:A:61:GLN:HG3  | 0.42     | 2.14        | 20     | 1     |
| 1:A:17:ILE:O    | 1:A:63:LEU:HD11 | 0.41     | 2.15        | 2      | 4     |
| 1:A:27:LYS:H    | 1:A:27:LYS:HE2  | 0.41     | 1.75        | 5      | 1     |
| 1:A:30:PRO:HA   | 1:A:34:CYS:HB2  | 0.41     | 1.93        | 4      | 1     |
| 1:A:46:ARG:HD3  | 1:A:46:ARG:H    | 0.41     | 1.76        | 4      | 1     |
| 1:A:16:LYS:HG2  | 1:A:59:TRP:CD1  | 0.41     | 2.50        | 17     | 1     |
| 1:A:40:LEU:HB3  | 1:A:50:GLU:HB3  | 0.40     | 1.93        | 11     | 1     |
| 1:A:26:ARG:HG3  | 1:A:50:GLU:OE2  | 0.40     | 2.15        | 4      | 1     |
| 1:A:49:ALA:O    | 1:A:51:LEU:HD12 | 0.40     | 2.17        | 1      | 1     |
| 1:A:28:GLN:HE21 | 1:A:38:ALA:HB3  | 0.40     | 1.76        | 9      | 1     |
| 1:A:16:LYS:HD2  | 1:A:59:TRP:NE1  | 0.40     | 2.32        | 15     | 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     | 62/113 (55%)    | 58±1 (94±2%) | 3±1 (5±2%) | 1±1 (1±1%) | 12          | 59 |
| All | All   | 1240/2260 (55%) | 1161 (94%)   | 62 (5%)    | 17 (1%)    | 12          | 59 |

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

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 33  | GLY  | 10             |
| 1   | A     | 8   | CYS  | 4              |
| 1   | A     | 30  | PRO  | 1              |
| 1   | A     | 9   | CYS  | 1              |
| 1   | A     | 13  | SER  | 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     | 58/96 (60%)     | 55±1 (94±2%) | 3±1 (6±2%) | 20          | 72 |
| All | All   | 1160/1920 (60%) | 1095 (94%)   | 65 (6%)    | 20          | 72 |

All 15 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     | 56  | LYS  | 17             |
| 1   | A     | 20  | LYS  | 14             |
| 1   | A     | 69  | LYS  | 6              |
| 1   | A     | 46  | ARG  | 5              |
| 1   | A     | 26  | ARG  | 5              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 16  | LYS  | 4              |
| 1   | A     | 15  | ARG  | 4              |
| 1   | A     | 27  | LYS  | 2              |
| 1   | A     | 11  | LYS  | 2              |
| 1   | A     | 36  | ILE  | 1              |
| 1   | A     | 64  | MET  | 1              |
| 1   | A     | 10  | LEU  | 1              |
| 1   | A     | 29  | GLU  | 1              |
| 1   | A     | 40  | LEU  | 1              |
| 1   | A     | 45  | LYS  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 83% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

|   |      |
|---|------|
| Total number of shifts                  | 1224 |
| Number of shifts mapped to atoms        | 811  |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 413  |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 4    |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 413 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 71  | PRO  | HA   | 4.5        | 0.02        | 1         |
| 1       | A     | 71  | PRO  | HB2  | 2.353      | 0.02        | 2         |
| 1       | A     | 71  | PRO  | HB3  | 1.966      | 0.02        | 2         |
| 1       | A     | 71  | PRO  | HD2  | 3.901      | 0.02        | 2         |
| 1       | A     | 71  | PRO  | HD3  | 3.76       | 0.02        | 2         |
| 1       | A     | 71  | PRO  | HG2  | 2.069      | 0.02        | 2         |
| 1       | A     | 71  | PRO  | HG3  | 2.069      | 0.02        | 2         |
| 1       | A     | 71  | PRO  | C    | 176.76     | 0.1         | 1         |
| 1       | A     | 71  | PRO  | CA   | 63.204     | 0.1         | 1         |
| 1       | A     | 71  | PRO  | CB   | 32.336     | 0.1         | 1         |
| 1       | A     | 71  | PRO  | CD   | 50.945     | 0.1         | 1         |
| 1       | A     | 71  | PRO  | CG   | 27.592     | 0.1         | 1         |
| 1       | A     | 72  | SER  | H    | 8.521      | 0.02        | 1         |
| 1       | A     | 72  | SER  | CA   | 56.652     | 0.1         | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 72  | SER  | CB   | 63.898     | 0.1         | 1         |
| 1       | A     | 72  | SER  | N    | 117.875    | 0.1         | 1         |
| 1       | A     | 73  | PRO  | HA   | 4.496      | 0.02        | 1         |
| 1       | A     | 73  | PRO  | HB2  | 2.362      | 0.02        | 2         |
| 1       | A     | 73  | PRO  | HB3  | 1.972      | 0.02        | 2         |
| 1       | A     | 73  | PRO  | HD2  | 3.987      | 0.02        | 2         |
| 1       | A     | 73  | PRO  | HD3  | 3.849      | 0.02        | 2         |
| 1       | A     | 73  | PRO  | HG2  | 2.079      | 0.02        | 2         |
| 1       | A     | 73  | PRO  | HG3  | 2.079      | 0.02        | 2         |
| 1       | A     | 73  | PRO  | C    | 176.862    | 0.1         | 1         |
| 1       | A     | 73  | PRO  | CA   | 63.457     | 0.1         | 1         |
| 1       | A     | 73  | PRO  | CB   | 32.336     | 0.1         | 1         |
| 1       | A     | 73  | PRO  | CD   | 51.036     | 0.1         | 1         |
| 1       | A     | 73  | PRO  | CG   | 27.592     | 0.1         | 1         |
| 1       | A     | 74  | GLN  | H    | 8.438      | 0.02        | 1         |
| 1       | A     | 74  | GLN  | HA   | 4.373      | 0.02        | 1         |
| 1       | A     | 74  | GLN  | HB2  | 2.113      | 0.02        | 2         |
| 1       | A     | 74  | GLN  | HB3  | 2.003      | 0.02        | 2         |
| 1       | A     | 74  | GLN  | HG2  | 2.445      | 0.02        | 2         |
| 1       | A     | 74  | GLN  | HG3  | 2.445      | 0.02        | 2         |
| 1       | A     | 74  | GLN  | C    | 175.841    | 0.1         | 1         |
| 1       | A     | 74  | GLN  | CA   | 55.766     | 0.1         | 1         |
| 1       | A     | 74  | GLN  | CB   | 29.964     | 0.1         | 1         |
| 1       | A     | 74  | GLN  | CG   | 33.978     | 0.1         | 1         |
| 1       | A     | 74  | GLN  | N    | 120.647    | 0.1         | 1         |
| 1       | A     | 75  | LYS  | H    | 8.415      | 0.02        | 1         |
| 1       | A     | 75  | LYS  | CA   | 54.451     | 0.1         | 1         |
| 1       | A     | 75  | LYS  | CB   | 32.883     | 0.1         | 1         |
| 1       | A     | 75  | LYS  | N    | 124.261    | 0.1         | 1         |
| 1       | A     | 76  | PRO  | HA   | 4.476      | 0.02        | 1         |
| 1       | A     | 76  | PRO  | HB2  | 2.324      | 0.02        | 2         |
| 1       | A     | 76  | PRO  | HB3  | 1.952      | 0.02        | 2         |
| 1       | A     | 76  | PRO  | HD2  | 3.879      | 0.02        | 2         |
| 1       | A     | 76  | PRO  | HD3  | 3.675      | 0.02        | 2         |
| 1       | A     | 76  | PRO  | HG2  | 2.069      | 0.02        | 2         |
| 1       | A     | 76  | PRO  | HG3  | 2.069      | 0.02        | 2         |
| 1       | A     | 76  | PRO  | C    | 176.658    | 0.1         | 1         |
| 1       | A     | 76  | PRO  | CA   | 63.204     | 0.1         | 1         |
| 1       | A     | 76  | PRO  | CB   | 32.336     | 0.1         | 1         |
| 1       | A     | 76  | PRO  | CD   | 50.58      | 0.1         | 1         |
| 1       | A     | 76  | PRO  | CG   | 27.684     | 0.1         | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 77  | ALA  | H    | 8.48       | 0.02        | 1         |
| 1       | A     | 77  | ALA  | HA   | 4.383      | 0.02        | 1         |
| 1       | A     | 77  | ALA  | HB1  | 1.427      | 0.02        | 1         |
| 1       | A     | 77  | ALA  | HB2  | 1.427      | 0.02        | 1         |
| 1       | A     | 77  | ALA  | HB3  | 1.427      | 0.02        | 1         |
| 1       | A     | 77  | ALA  | C    | 177.811    | 0.1         | 1         |
| 1       | A     | 77  | ALA  | CA   | 52.566     | 0.1         | 1         |
| 1       | A     | 77  | ALA  | CB   | 19.474     | 0.1         | 1         |
| 1       | A     | 77  | ALA  | N    | 124.618    | 0.1         | 1         |
| 1       | A     | 78  | GLN  | H    | 8.439      | 0.02        | 1         |
| 1       | A     | 78  | GLN  | HA   | 4.386      | 0.02        | 1         |
| 1       | A     | 78  | GLN  | HB2  | 2.157      | 0.02        | 2         |
| 1       | A     | 78  | GLN  | HB3  | 2.032      | 0.02        | 2         |
| 1       | A     | 78  | GLN  | HG2  | 2.436      | 0.02        | 2         |
| 1       | A     | 78  | GLN  | HG3  | 2.436      | 0.02        | 2         |
| 1       | A     | 78  | GLN  | C    | 176.483    | 0.1         | 1         |
| 1       | A     | 78  | GLN  | CA   | 56.078     | 0.1         | 1         |
| 1       | A     | 78  | GLN  | CB   | 30.055     | 0.1         | 1         |
| 1       | A     | 78  | GLN  | CG   | 33.978     | 0.1         | 1         |
| 1       | A     | 78  | GLN  | N    | 119.782    | 0.1         | 1         |
| 1       | A     | 79  | GLY  | H    | 8.446      | 0.02        | 1         |
| 1       | A     | 79  | GLY  | HA2  | 4.024      | 0.02        | 2         |
| 1       | A     | 79  | GLY  | HA3  | 4.024      | 0.02        | 2         |
| 1       | A     | 79  | GLY  | C    | 175.841    | 0.1         | 1         |
| 1       | A     | 79  | GLY  | CA   | 45.414     | 0.1         | 1         |
| 1       | A     | 79  | GLY  | N    | 109.652    | 0.1         | 1         |
| 1       | A     | 80  | CYS  | H    | 8.307      | 0.02        | 1         |
| 1       | A     | 80  | CYS  | HA   | 4.671      | 0.02        | 1         |
| 1       | A     | 80  | CYS  | HB2  | 2.745      | 0.02        | 2         |
| 1       | A     | 80  | CYS  | HB3  | 2.745      | 0.02        | 2         |
| 1       | A     | 80  | CYS  | C    | 176.308    | 0.1         | 1         |
| 1       | A     | 80  | CYS  | CA   | 55.759     | 0.1         | 1         |
| 1       | A     | 80  | CYS  | CB   | 41.914     | 0.1         | 1         |
| 1       | A     | 80  | CYS  | N    | 118.444    | 0.1         | 1         |
| 1       | A     | 81  | ARG  | H    | 8.373      | 0.02        | 1         |
| 1       | A     | 81  | ARG  | HA   | 4.404      | 0.02        | 1         |
| 1       | A     | 81  | ARG  | HB2  | 1.922      | 0.02        | 2         |
| 1       | A     | 81  | ARG  | HB3  | 1.828      | 0.02        | 2         |
| 1       | A     | 81  | ARG  | HD2  | 3.263      | 0.02        | 2         |
| 1       | A     | 81  | ARG  | HD3  | 3.263      | 0.02        | 2         |
| 1       | A     | 81  | ARG  | HG2  | 1.703      | 0.02        | 2         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 81  | ARG  | HG3  | 1.703      | 0.02        | 2         |
| 1       | A     | 81  | ARG  | C    | 176.249    | 0.1         | 1         |
| 1       | A     | 81  | ARG  | CA   | 56.49      | 0.1         | 1         |
| 1       | A     | 81  | ARG  | CB   | 31.15      | 0.1         | 1         |
| 1       | A     | 81  | ARG  | CD   | 43.83      | 0.1         | 1         |
| 1       | A     | 81  | ARG  | CG   | 27.227     | 0.1         | 1         |
| 1       | A     | 81  | ARG  | N    | 121.723    | 0.1         | 1         |
| 1       | A     | 82  | LYS  | H    | 8.455      | 0.02        | 1         |
| 1       | A     | 82  | LYS  | HA   | 4.364      | 0.02        | 1         |
| 1       | A     | 82  | LYS  | HB2  | 1.908      | 0.02        | 2         |
| 1       | A     | 82  | LYS  | HB3  | 1.807      | 0.02        | 2         |
| 1       | A     | 82  | LYS  | HD2  | 1.737      | 0.02        | 2         |
| 1       | A     | 82  | LYS  | HD3  | 1.737      | 0.02        | 2         |
| 1       | A     | 82  | LYS  | HE2  | 3.046      | 0.02        | 2         |
| 1       | A     | 82  | LYS  | HE3  | 3.046      | 0.02        | 2         |
| 1       | A     | 82  | LYS  | HG2  | 1.485      | 0.02        | 2         |
| 1       | A     | 82  | LYS  | HG3  | 1.485      | 0.02        | 2         |
| 1       | A     | 82  | LYS  | C    | 176.191    | 0.1         | 1         |
| 1       | A     | 82  | LYS  | CA   | 56.734     | 0.1         | 1         |
| 1       | A     | 82  | LYS  | CB   | 33.066     | 0.1         | 1         |
| 1       | A     | 82  | LYS  | CD   | 29.573     | 0.1         | 1         |
| 1       | A     | 82  | LYS  | CE   | 42.515     | 0.1         | 1         |
| 1       | A     | 82  | LYS  | CG   | 25.043     | 0.1         | 1         |
| 1       | A     | 82  | LYS  | N    | 122.697    | 0.1         | 1         |
| 1       | A     | 83  | ASP  | H    | 8.362      | 0.02        | 1         |
| 1       | A     | 83  | ASP  | CA   | 54.299     | 0.1         | 1         |
| 1       | A     | 83  | ASP  | CB   | 41.64      | 0.1         | 1         |
| 1       | A     | 83  | ASP  | N    | 121.227    | 0.1         | 1         |
| 1       | A     | 84  | ARG  | HA   | 4.373      | 0.02        | 1         |
| 1       | A     | 84  | ARG  | HB2  | 1.982      | 0.02        | 2         |
| 1       | A     | 84  | ARG  | HB3  | 1.88       | 0.02        | 2         |
| 1       | A     | 84  | ARG  | HD2  | 3.259      | 0.02        | 2         |
| 1       | A     | 84  | ARG  | HD3  | 3.259      | 0.02        | 2         |
| 1       | A     | 84  | ARG  | HG2  | 1.701      | 0.02        | 2         |
| 1       | A     | 84  | ARG  | HG3  | 1.701      | 0.02        | 2         |
| 1       | A     | 84  | ARG  | C    | 176.979    | 0.1         | 1         |
| 1       | A     | 84  | ARG  | CA   | 56.734     | 0.1         | 1         |
| 1       | A     | 84  | ARG  | CB   | 30.694     | 0.1         | 1         |
| 1       | A     | 84  | ARG  | CD   | 43.83      | 0.1         | 1         |
| 1       | A     | 84  | ARG  | CG   | 27.136     | 0.1         | 1         |
| 1       | A     | 85  | GLY  | H    | 8.494      | 0.02        | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 85  | GLY  | HA2  | 3.993      | 0.02        | 2         |
| 1       | A     | 85  | GLY  | HA3  | 3.993      | 0.02        | 2         |
| 1       | A     | 85  | GLY  | C    | 174.075    | 0.1         | 1         |
| 1       | A     | 85  | GLY  | CA   | 45.468     | 0.1         | 1         |
| 1       | A     | 85  | GLY  | N    | 109.402    | 0.1         | 1         |
| 1       | A     | 86  | ALA  | H    | 8.145      | 0.02        | 1         |
| 1       | A     | 86  | ALA  | HA   | 4.372      | 0.02        | 1         |
| 1       | A     | 86  | ALA  | HB1  | 1.449      | 0.02        | 1         |
| 1       | A     | 86  | ALA  | HB2  | 1.449      | 0.02        | 1         |
| 1       | A     | 86  | ALA  | HB3  | 1.449      | 0.02        | 1         |
| 1       | A     | 86  | ALA  | C    | 178.001    | 0.1         | 1         |
| 1       | A     | 86  | ALA  | CA   | 52.834     | 0.1         | 1         |
| 1       | A     | 86  | ALA  | CB   | 19.565     | 0.1         | 1         |
| 1       | A     | 86  | ALA  | N    | 123.603    | 0.1         | 1         |
| 1       | A     | 87  | SER  | H    | 8.316      | 0.02        | 1         |
| 1       | A     | 87  | SER  | HA   | 4.517      | 0.02        | 1         |
| 1       | A     | 87  | SER  | HB2  | 3.922      | 0.02        | 2         |
| 1       | A     | 87  | SER  | HB3  | 3.922      | 0.02        | 2         |
| 1       | A     | 87  | SER  | C    | 174.849    | 0.1         | 1         |
| 1       | A     | 87  | SER  | CA   | 58.629     | 0.1         | 1         |
| 1       | A     | 87  | SER  | CB   | 64.126     | 0.1         | 1         |
| 1       | A     | 87  | SER  | N    | 114.782    | 0.1         | 1         |
| 1       | A     | 88  | LYS  | H    | 8.482      | 0.02        | 1         |
| 1       | A     | 88  | LYS  | HA   | 4.424      | 0.02        | 1         |
| 1       | A     | 88  | LYS  | HB2  | 1.952      | 0.02        | 2         |
| 1       | A     | 88  | LYS  | HB3  | 1.838      | 0.02        | 2         |
| 1       | A     | 88  | LYS  | HD2  | 1.741      | 0.02        | 2         |
| 1       | A     | 88  | LYS  | HD3  | 1.741      | 0.02        | 2         |
| 1       | A     | 88  | LYS  | HE2  | 3.035      | 0.02        | 2         |
| 1       | A     | 88  | LYS  | HE3  | 3.035      | 0.02        | 2         |
| 1       | A     | 88  | LYS  | HG2  | 1.53       | 0.02        | 2         |
| 1       | A     | 88  | LYS  | HG3  | 1.53       | 0.02        | 2         |
| 1       | A     | 88  | LYS  | C    | 177.037    | 0.1         | 1         |
| 1       | A     | 88  | LYS  | CA   | 57.059     | 0.1         | 1         |
| 1       | A     | 88  | LYS  | CB   | 33.066     | 0.1         | 1         |
| 1       | A     | 88  | LYS  | CD   | 29.326     | 0.1         | 1         |
| 1       | A     | 88  | LYS  | CG   | 25.129     | 0.1         | 1         |
| 1       | A     | 88  | LYS  | N    | 123.133    | 0.1         | 1         |
| 1       | A     | 89  | THR  | H    | 8.061      | 0.02        | 1         |
| 1       | A     | 89  | THR  | HA   | 4.383      | 0.02        | 1         |
| 1       | A     | 89  | THR  | HB   | 4.289      | 0.02        | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 89  | THR  | HG21 | 1.244      | 0.02        | 1         |
| 1       | A     | 89  | THR  | HG22 | 1.244      | 0.02        | 1         |
| 1       | A     | 89  | THR  | HG23 | 1.244      | 0.02        | 1         |
| 1       | A     | 89  | THR  | C    | 175.199    | 0.1         | 1         |
| 1       | A     | 89  | THR  | CA   | 61.96      | 0.1         | 1         |
| 1       | A     | 89  | THR  | CB   | 70.283     | 0.1         | 1         |
| 1       | A     | 89  | THR  | CG2  | 21.754     | 0.1         | 1         |
| 1       | A     | 89  | THR  | N    | 112.586    | 0.1         | 1         |
| 1       | A     | 90  | GLY  | H    | 8.315      | 0.02        | 1         |
| 1       | A     | 90  | GLY  | HA2  | 4.226      | 0.02        | 2         |
| 1       | A     | 90  | GLY  | HA3  | 4.226      | 0.02        | 2         |
| 1       | A     | 90  | GLY  | C    | 174.192    | 0.1         | 1         |
| 1       | A     | 90  | GLY  | CA   | 45.414     | 0.1         | 1         |
| 1       | A     | 90  | GLY  | N    | 110.812    | 0.1         | 1         |
| 1       | A     | 91  | LYS  | H    | 8.219      | 0.02        | 1         |
| 1       | A     | 91  | LYS  | HA   | 4.384      | 0.02        | 1         |
| 1       | A     | 91  | LYS  | HB2  | 1.85       | 0.02        | 2         |
| 1       | A     | 91  | LYS  | HB3  | 1.482      | 0.02        | 2         |
| 1       | A     | 91  | LYS  | HD2  | 1.72       | 0.02        | 2         |
| 1       | A     | 91  | LYS  | HD3  | 1.72       | 0.02        | 2         |
| 1       | A     | 91  | LYS  | HE2  | 3.044      | 0.02        | 2         |
| 1       | A     | 91  | LYS  | HE3  | 3.044      | 0.02        | 2         |
| 1       | A     | 91  | LYS  | HG2  | 1.482      | 0.02        | 2         |
| 1       | A     | 91  | LYS  | HG3  | 1.482      | 0.02        | 2         |
| 1       | A     | 91  | LYS  | C    | 176.848    | 0.1         | 1         |
| 1       | A     | 91  | LYS  | CA   | 56.544     | 0.1         | 1         |
| 1       | A     | 91  | LYS  | CB   | 33.339     | 0.1         | 1         |
| 1       | A     | 91  | LYS  | CD   | 29.573     | 0.1         | 1         |
| 1       | A     | 91  | LYS  | CE   | 42.191     | 0.1         | 1         |
| 1       | A     | 91  | LYS  | CG   | 25.043     | 0.1         | 1         |
| 1       | A     | 91  | LYS  | N    | 120.822    | 0.1         | 1         |
| 1       | A     | 92  | LYS  | H    | 8.426      | 0.02        | 1         |
| 1       | A     | 92  | LYS  | HA   | 4.383      | 0.02        | 1         |
| 1       | A     | 92  | LYS  | HB2  | 1.88       | 0.02        | 2         |
| 1       | A     | 92  | LYS  | HB3  | 1.88       | 0.02        | 2         |
| 1       | A     | 92  | LYS  | HD2  | 1.728      | 0.02        | 2         |
| 1       | A     | 92  | LYS  | HD3  | 1.728      | 0.02        | 2         |
| 1       | A     | 92  | LYS  | HE2  | 3.045      | 0.02        | 2         |
| 1       | A     | 92  | LYS  | HE3  | 3.045      | 0.02        | 2         |
| 1       | A     | 92  | LYS  | HG2  | 1.499      | 0.02        | 2         |
| 1       | A     | 92  | LYS  | HG3  | 1.499      | 0.02        | 2         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 92  | LYS  | C    | 177.081    | 0.1         | 1         |
| 1       | A     | 92  | LYS  | CA   | 56.707     | 0.1         | 1         |
| 1       | A     | 92  | LYS  | CB   | 33.157     | 0.1         | 1         |
| 1       | A     | 92  | LYS  | CD   | 29.417     | 0.1         | 1         |
| 1       | A     | 92  | LYS  | CG   | 25.038     | 0.1         | 1         |
| 1       | A     | 92  | LYS  | N    | 122.06     | 0.1         | 1         |
| 1       | A     | 93  | GLY  | H    | 8.385      | 0.02        | 1         |
| 1       | A     | 93  | GLY  | HA2  | 4.034      | 0.02        | 2         |
| 1       | A     | 93  | GLY  | HA3  | 4.034      | 0.02        | 2         |
| 1       | A     | 93  | GLY  | C    | 174.177    | 0.1         | 1         |
| 1       | A     | 93  | GLY  | CA   | 45.36      | 0.1         | 1         |
| 1       | A     | 93  | GLY  | N    | 109.899    | 0.1         | 1         |
| 1       | A     | 94  | LYS  | H    | 8.329      | 0.02        | 1         |
| 1       | A     | 94  | LYS  | HA   | 4.404      | 0.02        | 1         |
| 1       | A     | 94  | LYS  | HB2  | 1.874      | 0.02        | 2         |
| 1       | A     | 94  | LYS  | HB3  | 1.874      | 0.02        | 2         |
| 1       | A     | 94  | LYS  | HD2  | 1.736      | 0.02        | 2         |
| 1       | A     | 94  | LYS  | HD3  | 1.736      | 0.02        | 2         |
| 1       | A     | 94  | LYS  | HE2  | 3.055      | 0.02        | 2         |
| 1       | A     | 94  | LYS  | HE3  | 3.055      | 0.02        | 2         |
| 1       | A     | 94  | LYS  | HG2  | 1.499      | 0.02        | 2         |
| 1       | A     | 94  | LYS  | HG3  | 1.499      | 0.02        | 2         |
| 1       | A     | 94  | LYS  | C    | 176.571    | 0.1         | 1         |
| 1       | A     | 94  | LYS  | CA   | 56.666     | 0.1         | 1         |
| 1       | A     | 94  | LYS  | CB   | 33.522     | 0.1         | 1         |
| 1       | A     | 94  | LYS  | CD   | 29.417     | 0.1         | 1         |
| 1       | A     | 94  | LYS  | CE   | 43.83      | 0.1         | 1         |
| 1       | A     | 94  | LYS  | CG   | 25.129     | 0.1         | 1         |
| 1       | A     | 94  | LYS  | N    | 120.98     | 0.1         | 1         |
| 1       | A     | 95  | GLY  | H    | 8.536      | 0.02        | 1         |
| 1       | A     | 95  | GLY  | HA2  | 4.055      | 0.02        | 2         |
| 1       | A     | 95  | GLY  | HA3  | 4.055      | 0.02        | 2         |
| 1       | A     | 95  | GLY  | C    | 174.206    | 0.1         | 1         |
| 1       | A     | 95  | GLY  | CA   | 45.387     | 0.1         | 1         |
| 1       | A     | 95  | GLY  | N    | 109.962    | 0.1         | 1         |
| 1       | A     | 96  | SER  | H    | 8.254      | 0.02        | 1         |
| 1       | A     | 96  | SER  | HA   | 4.517      | 0.02        | 1         |
| 1       | A     | 96  | SER  | HB2  | 3.942      | 0.02        | 2         |
| 1       | A     | 96  | SER  | HB3  | 3.942      | 0.02        | 2         |
| 1       | A     | 96  | SER  | C    | 174.396    | 0.1         | 1         |
| 1       | A     | 96  | SER  | CA   | 58.508     | 0.1         | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 96  | SER  | CB   | 64.308     | 0.1         | 1         |
| 1       | A     | 96  | SER  | N    | 115.623    | 0.1         | 1         |
| 1       | A     | 97  | LYS  | H    | 8.491      | 0.02        | 1         |
| 1       | A     | 97  | LYS  | HA   | 4.404      | 0.02        | 1         |
| 1       | A     | 97  | LYS  | HB2  | 1.868      | 0.02        | 2         |
| 1       | A     | 97  | LYS  | HB3  | 1.868      | 0.02        | 2         |
| 1       | A     | 97  | LYS  | HD2  | 1.721      | 0.02        | 2         |
| 1       | A     | 97  | LYS  | HD3  | 1.721      | 0.02        | 2         |
| 1       | A     | 97  | LYS  | HE2  | 3.034      | 0.02        | 2         |
| 1       | A     | 97  | LYS  | HE3  | 3.034      | 0.02        | 2         |
| 1       | A     | 97  | LYS  | HG2  | 1.469      | 0.02        | 2         |
| 1       | A     | 97  | LYS  | HG3  | 1.469      | 0.02        | 2         |
| 1       | A     | 97  | LYS  | C    | 177.081    | 0.1         | 1         |
| 1       | A     | 97  | LYS  | CA   | 56.815     | 0.1         | 1         |
| 1       | A     | 97  | LYS  | CB   | 33.248     | 0.1         | 1         |
| 1       | A     | 97  | LYS  | CD   | 29.417     | 0.1         | 1         |
| 1       | A     | 97  | LYS  | CG   | 25.129     | 0.1         | 1         |
| 1       | A     | 97  | LYS  | N    | 123.441    | 0.1         | 1         |
| 1       | A     | 98  | GLY  | H    | 8.435      | 0.02        | 1         |
| 1       | A     | 98  | GLY  | HA2  | 4.034      | 0.02        | 2         |
| 1       | A     | 98  | GLY  | HA3  | 4.034      | 0.02        | 2         |
| 1       | A     | 98  | GLY  | C    | 173.958    | 0.1         | 1         |
| 1       | A     | 98  | GLY  | CA   | 45.414     | 0.1         | 1         |
| 1       | A     | 98  | GLY  | N    | 109.184    | 0.1         | 1         |
| 1       | A     | 99  | CYS  | H    | 8.413      | 0.02        | 1         |
| 1       | A     | 99  | CYS  | HA   | 4.414      | 0.02        | 1         |
| 1       | A     | 99  | CYS  | HB2  | 3.275      | 0.02        | 2         |
| 1       | A     | 99  | CYS  | HB3  | 3.07       | 0.02        | 2         |
| 1       | A     | 99  | CYS  | C    | 174.469    | 0.1         | 1         |
| 1       | A     | 99  | CYS  | CA   | 55.732     | 0.1         | 1         |
| 1       | A     | 99  | CYS  | CB   | 41.777     | 0.1         | 1         |
| 1       | A     | 99  | CYS  | N    | 118.609    | 0.1         | 1         |
| 1       | A     | 100 | LYS  | H    | 8.496      | 0.02        | 1         |
| 1       | A     | 100 | LYS  | HA   | 4.381      | 0.02        | 1         |
| 1       | A     | 100 | LYS  | HB2  | 1.88       | 0.02        | 2         |
| 1       | A     | 100 | LYS  | HB3  | 1.88       | 0.02        | 2         |
| 1       | A     | 100 | LYS  | HD2  | 1.737      | 0.02        | 2         |
| 1       | A     | 100 | LYS  | HD3  | 1.737      | 0.02        | 2         |
| 1       | A     | 100 | LYS  | HE2  | 3.066      | 0.02        | 2         |
| 1       | A     | 100 | LYS  | HE3  | 3.066      | 0.02        | 2         |
| 1       | A     | 100 | LYS  | HG2  | 1.489      | 0.02        | 2         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 100 | LYS  | HG3  | 1.489      | 0.02        | 2         |
| 1       | A     | 100 | LYS  | C    | 176.264    | 0.1         | 1         |
| 1       | A     | 100 | LYS  | CA   | 56.463     | 0.1         | 1         |
| 1       | A     | 100 | LYS  | CB   | 33.43      | 0.1         | 1         |
| 1       | A     | 100 | LYS  | CD   | 29.599     | 0.1         | 1         |
| 1       | A     | 100 | LYS  | CE   | 41.64      | 0.1         | 1         |
| 1       | A     | 100 | LYS  | CG   | 25.038     | 0.1         | 1         |
| 1       | A     | 100 | LYS  | N    | 123.629    | 0.1         | 1         |
| 1       | A     | 101 | ARG  | H    | 8.509      | 0.02        | 1         |
| 1       | A     | 101 | ARG  | HA   | 4.407      | 0.02        | 1         |
| 1       | A     | 101 | ARG  | HB2  | 1.925      | 0.02        | 2         |
| 1       | A     | 101 | ARG  | HB3  | 1.825      | 0.02        | 2         |
| 1       | A     | 101 | ARG  | HD2  | 3.259      | 0.02        | 2         |
| 1       | A     | 101 | ARG  | HD3  | 3.259      | 0.02        | 2         |
| 1       | A     | 101 | ARG  | HG2  | 1.703      | 0.02        | 2         |
| 1       | A     | 101 | ARG  | HG3  | 1.703      | 0.02        | 2         |
| 1       | A     | 101 | ARG  | C    | 176.439    | 0.1         | 1         |
| 1       | A     | 101 | ARG  | CA   | 56.416     | 0.1         | 1         |
| 1       | A     | 101 | ARG  | CB   | 31.15      | 0.1         | 1         |
| 1       | A     | 101 | ARG  | CD   | 43.83      | 0.1         | 1         |
| 1       | A     | 101 | ARG  | CG   | 27.319     | 0.1         | 1         |
| 1       | A     | 101 | ARG  | N    | 123.442    | 0.1         | 1         |
| 1       | A     | 102 | THR  | H    | 8.286      | 0.02        | 1         |
| 1       | A     | 102 | THR  | HA   | 4.383      | 0.02        | 1         |
| 1       | A     | 102 | THR  | HB   | 4.3        | 0.02        | 1         |
| 1       | A     | 102 | THR  | HG21 | 1.239      | 0.02        | 1         |
| 1       | A     | 102 | THR  | HG22 | 1.239      | 0.02        | 1         |
| 1       | A     | 102 | THR  | HG23 | 1.239      | 0.02        | 1         |
| 1       | A     | 102 | THR  | C    | 174.498    | 0.1         | 1         |
| 1       | A     | 102 | THR  | CA   | 62.069     | 0.1         | 1         |
| 1       | A     | 102 | THR  | CB   | 70.238     | 0.1         | 1         |
| 1       | A     | 102 | THR  | CG2  | 21.754     | 0.1         | 1         |
| 1       | A     | 102 | THR  | N    | 116.093    | 0.1         | 1         |
| 1       | A     | 103 | GLU  | H    | 8.523      | 0.02        | 1         |
| 1       | A     | 103 | GLU  | HA   | 4.388      | 0.02        | 1         |
| 1       | A     | 103 | GLU  | HB2  | 2.095      | 0.02        | 2         |
| 1       | A     | 103 | GLU  | HB3  | 1.98       | 0.02        | 2         |
| 1       | A     | 103 | GLU  | HG2  | 2.323      | 0.02        | 2         |
| 1       | A     | 103 | GLU  | HG3  | 2.323      | 0.02        | 2         |
| 1       | A     | 103 | GLU  | C    | 176.352    | 0.1         | 1         |
| 1       | A     | 103 | GLU  | CA   | 56.598     | 0.1         | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 103 | GLU  | CB   | 30.603     | 0.1         | 1         |
| 1       | A     | 103 | GLU  | CG   | 36.441     | 0.1         | 1         |
| 1       | A     | 103 | GLU  | N    | 124.044    | 0.1         | 1         |
| 1       | A     | 104 | ARG  | H    | 8.487      | 0.02        | 1         |
| 1       | A     | 104 | ARG  | HA   | 4.396      | 0.02        | 1         |
| 1       | A     | 104 | ARG  | HB2  | 1.927      | 0.02        | 2         |
| 1       | A     | 104 | ARG  | HB3  | 1.825      | 0.02        | 2         |
| 1       | A     | 104 | ARG  | HD2  | 3.249      | 0.02        | 2         |
| 1       | A     | 104 | ARG  | HD3  | 3.249      | 0.02        | 2         |
| 1       | A     | 104 | ARG  | HG2  | 1.668      | 0.02        | 2         |
| 1       | A     | 104 | ARG  | HG3  | 1.668      | 0.02        | 2         |
| 1       | A     | 104 | ARG  | C    | 176.352    | 0.1         | 1         |
| 1       | A     | 104 | ARG  | CA   | 56.382     | 0.1         | 1         |
| 1       | A     | 104 | ARG  | CB   | 31.515     | 0.1         | 1         |
| 1       | A     | 104 | ARG  | CD   | 43.647     | 0.1         | 1         |
| 1       | A     | 104 | ARG  | CG   | 27.136     | 0.1         | 1         |
| 1       | A     | 104 | ARG  | N    | 122.268    | 0.1         | 1         |
| 1       | A     | 105 | SER  | H    | 8.415      | 0.02        | 1         |
| 1       | A     | 105 | SER  | HA   | 4.476      | 0.02        | 1         |
| 1       | A     | 105 | SER  | HB2  | 3.911      | 0.02        | 2         |
| 1       | A     | 105 | SER  | HB3  | 3.911      | 0.02        | 2         |
| 1       | A     | 105 | SER  | C    | 174.484    | 0.1         | 1         |
| 1       | A     | 105 | SER  | CA   | 58.562     | 0.1         | 1         |
| 1       | A     | 105 | SER  | CB   | 64.126     | 0.1         | 1         |
| 1       | A     | 105 | SER  | N    | 117.275    | 0.1         | 1         |
| 1       | A     | 106 | GLN  | H    | 8.506      | 0.02        | 1         |
| 1       | A     | 106 | GLN  | HA   | 4.486      | 0.02        | 1         |
| 1       | A     | 106 | GLN  | HB2  | 2.188      | 0.02        | 2         |
| 1       | A     | 106 | GLN  | HB3  | 2.023      | 0.02        | 2         |
| 1       | A     | 106 | GLN  | HG2  | 2.415      | 0.02        | 2         |
| 1       | A     | 106 | GLN  | HG3  | 2.415      | 0.02        | 2         |
| 1       | A     | 106 | GLN  | C    | 175.841    | 0.1         | 1         |
| 1       | A     | 106 | GLN  | CA   | 55.813     | 0.1         | 1         |
| 1       | A     | 106 | GLN  | CB   | 29.964     | 0.1         | 1         |
| 1       | A     | 106 | GLN  | CG   | 33.978     | 0.1         | 1         |
| 1       | A     | 106 | GLN  | N    | 122.267    | 0.1         | 1         |
| 1       | A     | 107 | THR  | H    | 8.297      | 0.02        | 1         |
| 1       | A     | 107 | THR  | CA   | 60.092     | 0.1         | 1         |
| 1       | A     | 107 | THR  | CB   | 70.101     | 0.1         | 1         |
| 1       | A     | 107 | THR  | N    | 118.211    | 0.1         | 1         |
| 1       | A     | 108 | PRO  | HA   | 4.486      | 0.02        | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 108 | PRO  | HB2  | 2.34       | 0.02        | 2         |
| 1       | A     | 108 | PRO  | HB3  | 1.957      | 0.02        | 2         |
| 1       | A     | 108 | PRO  | HD2  | 3.906      | 0.02        | 2         |
| 1       | A     | 108 | PRO  | HD3  | 3.76       | 0.02        | 2         |
| 1       | A     | 108 | PRO  | HG2  | 2.059      | 0.02        | 2         |
| 1       | A     | 108 | PRO  | HG3  | 2.059      | 0.02        | 2         |
| 1       | A     | 108 | PRO  | C    | 176.862    | 0.1         | 1         |
| 1       | A     | 108 | PRO  | CA   | 63.504     | 0.1         | 1         |
| 1       | A     | 108 | PRO  | CB   | 32.485     | 0.1         | 1         |
| 1       | A     | 108 | PRO  | CD   | 51.31      | 0.1         | 1         |
| 1       | A     | 108 | PRO  | CG   | 27.775     | 0.1         | 1         |
| 1       | A     | 109 | LYS  | H    | 8.453      | 0.02        | 1         |
| 1       | A     | 109 | LYS  | HA   | 4.383      | 0.02        | 1         |
| 1       | A     | 109 | LYS  | HB2  | 1.88       | 0.02        | 2         |
| 1       | A     | 109 | LYS  | HB3  | 1.88       | 0.02        | 2         |
| 1       | A     | 109 | LYS  | HD2  | 1.735      | 0.02        | 2         |
| 1       | A     | 109 | LYS  | HD3  | 1.735      | 0.02        | 2         |
| 1       | A     | 109 | LYS  | HE2  | 3.106      | 0.02        | 2         |
| 1       | A     | 109 | LYS  | HE3  | 3.106      | 0.02        | 2         |
| 1       | A     | 109 | LYS  | HG2  | 1.495      | 0.02        | 2         |
| 1       | A     | 109 | LYS  | HG3  | 1.495      | 0.02        | 2         |
| 1       | A     | 109 | LYS  | C    | 176.731    | 0.1         | 1         |
| 1       | A     | 109 | LYS  | CA   | 56.463     | 0.1         | 1         |
| 1       | A     | 109 | LYS  | CB   | 33.522     | 0.1         | 1         |
| 1       | A     | 109 | LYS  | CD   | 29.234     | 0.1         | 1         |
| 1       | A     | 109 | LYS  | CG   | 25.038     | 0.1         | 1         |
| 1       | A     | 109 | LYS  | N    | 121.556    | 0.1         | 1         |
| 1       | A     | 110 | GLY  | H    | 8.213      | 0.02        | 1         |
| 1       | A     | 110 | GLY  | CA   | 44.222     | 0.1         | 1         |
| 1       | A     | 110 | GLY  | N    | 110.094    | 0.1         | 1         |

### 7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 109      | $-0.09 \pm 0.28$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 99       | $-0.10 \pm 0.23$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 98       | $-0.06 \pm 0.11$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 98       | $0.09 \pm 0.45$                 | None needed ( $< 0.5$ ppm) |

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 765 atoms were assigned a chemical shift out of a possible 916. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 295/306 (96%) | 117/122 (96%)  | 120/126 (95%)   | 58/58 (100%)    |
| Sidechain | 438/562 (78%) | 297/364 (82%)  | 141/170 (83%)   | 0/28 (0%)       |
| Aromatic  | 32/48 (67%)   | 18/23 (78%)    | 13/22 (59%)     | 1/3 (33%)       |
| Overall   | 765/916 (84%) | 432/509 (85%)  | 274/318 (86%)   | 59/89 (66%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 811 atoms were assigned a chemical shift out of a possible 978. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 325/343 (95%) | 130/138 (94%)  | 132/140 (94%)   | 63/65 (97%)     |
| Sidechain | 454/587 (77%) | 308/379 (81%)  | 146/179 (82%)   | 0/29 (0%)       |
| Aromatic  | 32/48 (67%)   | 18/23 (78%)    | 13/22 (59%)     | 1/3 (33%)       |
| Overall   | 811/978 (83%) | 456/540 (84%)  | 291/341 (85%)   | 64/97 (66%)     |

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

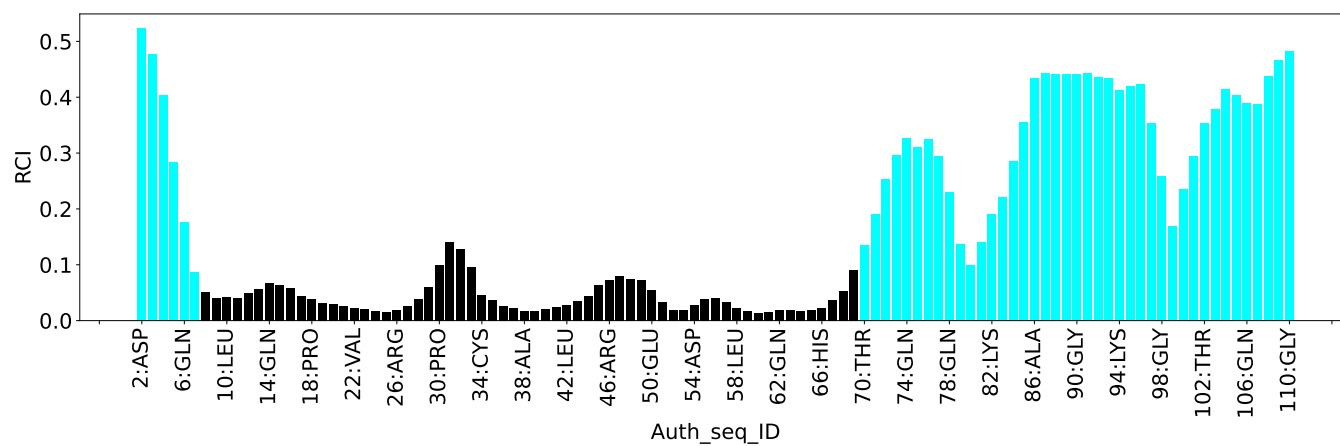
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 39  | ILE  | CG2  | 9.51       | 10.93 – 24.12       | -6.1    |
| 1       | A     | 60  | VAL  | HG21 | -0.59      | -0.58 – 2.19        | -5.0    |
| 1       | A     | 60  | VAL  | HG22 | -0.59      | -0.58 – 2.19        | -5.0    |
| 1       | A     | 60  | VAL  | HG23 | -0.59      | -0.58 – 2.19        | -5.0    |

### 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                                | 592   |
| Intra-residue ( $ i-j =0$ )                              | 265   |
| Sequential ( $ i-j =1$ )                                 | 150   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 54    |
| Long range ( $ i-j \geq 5$ )                             | 121   |
| Inter-chain  | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 2     |
| Total dihedral-angle restraints                          | 89    |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 6.0   |
| Number of long range restraints per residue <sup>1</sup> | 1.1   |

<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)  | 10.8                                   | 0.2     |
| 0.2-0.5 (Medium) | 3.5                                    | 0.4     |
| >0.5 (Large)     | None                                   | None    |

### 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)   | 7.3                                    | 3.15    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis [i](#)

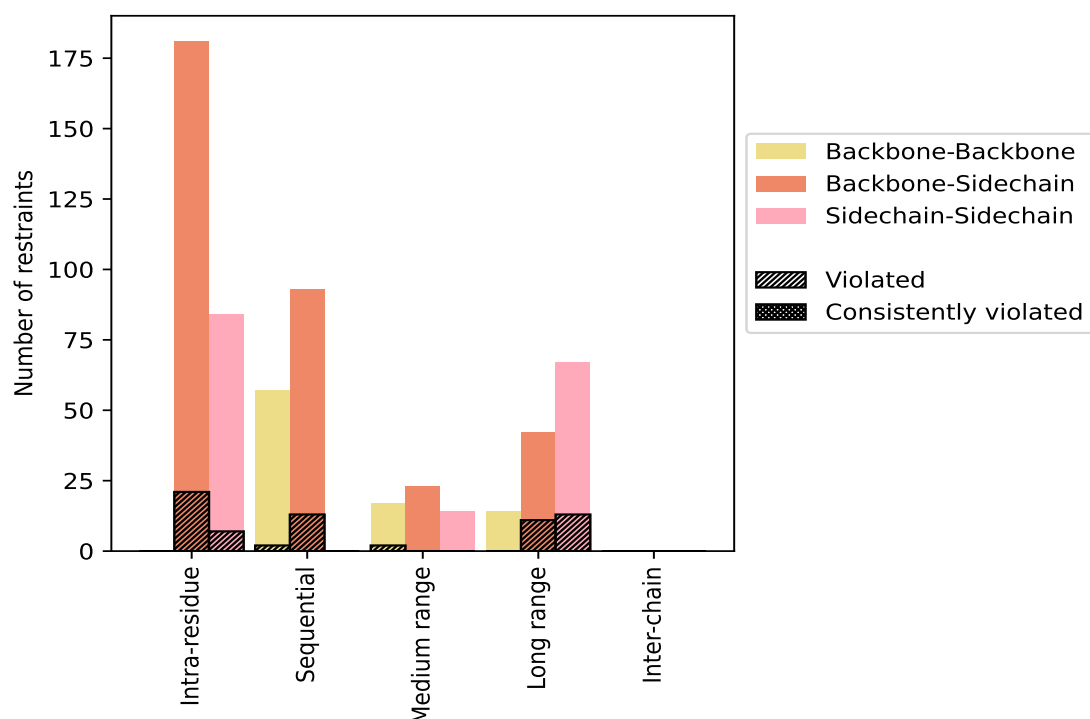
### 9.1 Summary of distance violations [i](#)

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.

| Restraints 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="#">265</a> | <a href="#">44.8</a>  | <a href="#">28</a>    | <a href="#">10.6</a> | <a href="#">4.7</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   | 181                 | 30.6                  | 21                    | 11.6                 | 3.5                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain  | 84                  | 14.2                  | 7                     | 8.3                  | 1.2                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">150</a> | <a href="#">25.3</a>  | <a href="#">15</a>    | <a href="#">10.0</a> | <a href="#">2.5</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone  | 57                  | 9.6                   | 2                     | 3.5                  | 0.3                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain   | 93                  | 15.7                  | 13                    | 14.0                 | 2.2                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain  | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">54</a>  | <a href="#">9.1</a>   | <a href="#">2</a>     | <a href="#">3.7</a>  | <a href="#">0.3</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone  | 17                  | 2.9                   | 2                     | 11.8                 | 0.3                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain   | 23                  | 3.9                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain  | 14                  | 2.4                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">121</a> | <a href="#">20.4</a>  | <a href="#">24</a>    | <a href="#">19.8</a> | <a href="#">4.1</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone  | 14                  | 2.4                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain   | 42                  | 7.1                   | 11                    | 26.2                 | 1.9                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain  | 65                  | 11.0                  | 13                    | 20.0                 | 2.2                  | 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="#">2</a>   | <a href="#">0.3</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="#">592</a> | <a href="#">100.0</a> | <a href="#">69</a>    | <a href="#">11.7</a> | <a href="#">11.7</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone  | 88                  | 14.9                  | 4                     | 4.5                  | 0.7                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain   | 339                 | 57.3                  | 45                    | 13.3                 | 7.6                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain  | 165                 | 27.9                  | 20                    | 12.1                 | 3.4                  | 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        | 8                    | 2               | 1               | 4               | 0               | 15    | 0.17     | 0.26    | 0.06                | 0.14       |
| 2        | 7                    | 3               | 2               | 4               | 0               | 16    | 0.17     | 0.3     | 0.05                | 0.14       |
| 3        | 7                    | 4               | 0               | 4               | 0               | 15    | 0.15     | 0.3     | 0.05                | 0.12       |
| 4        | 8                    | 1               | 1               | 3               | 0               | 13    | 0.17     | 0.3     | 0.06                | 0.18       |
| 5        | 5                    | 3               | 1               | 6               | 0               | 15    | 0.16     | 0.29    | 0.05                | 0.15       |
| 6        | 7                    | 6               | 1               | 6               | 0               | 20    | 0.16     | 0.31    | 0.06                | 0.14       |
| 7        | 8                    | 7               | 2               | 2               | 0               | 19    | 0.15     | 0.27    | 0.05                | 0.14       |
| 8        | 6                    | 3               | 1               | 3               | 0               | 13    | 0.16     | 0.27    | 0.05                | 0.15       |
| 9        | 8                    | 4               | 2               | 3               | 0               | 17    | 0.16     | 0.29    | 0.05                | 0.13       |
| 10       | 6                    | 4               | 1               | 3               | 0               | 14    | 0.17     | 0.29    | 0.06                | 0.16       |

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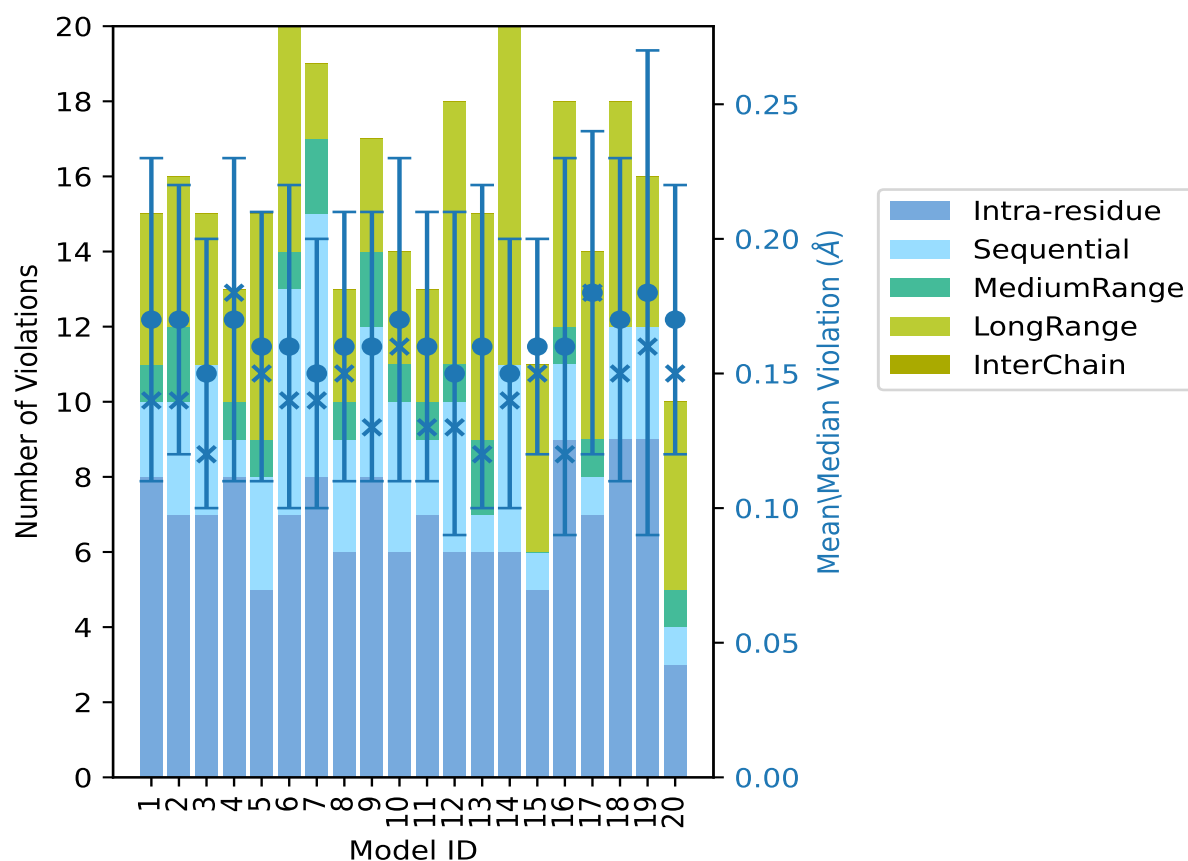
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 7                    | 2               | 1               | 3               | 0               | 13    | 0.16     | 0.27    | 0.05                | 0.13       |
| 12       | 6                    | 4               | 1               | 7               | 0               | 18    | 0.15     | 0.31    | 0.06                | 0.13       |
| 13       | 6                    | 1               | 2               | 6               | 0               | 15    | 0.16     | 0.29    | 0.06                | 0.12       |
| 14       | 6                    | 5               | 0               | 9               | 0               | 20    | 0.15     | 0.24    | 0.05                | 0.14       |
| 15       | 5                    | 1               | 0               | 5               | 0               | 11    | 0.16     | 0.26    | 0.04                | 0.15       |
| 16       | 9                    | 2               | 1               | 6               | 0               | 18    | 0.16     | 0.32    | 0.07                | 0.12       |
| 17       | 7                    | 1               | 1               | 5               | 0               | 14    | 0.18     | 0.3     | 0.06                | 0.18       |
| 18       | 9                    | 3               | 0               | 6               | 0               | 18    | 0.17     | 0.3     | 0.06                | 0.15       |
| 19       | 9                    | 3               | 0               | 4               | 0               | 16    | 0.18     | 0.4     | 0.09                | 0.16       |
| 20       | 3                    | 1               | 1               | 5               | 0               | 10    | 0.17     | 0.28    | 0.05                | 0.15       |

<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

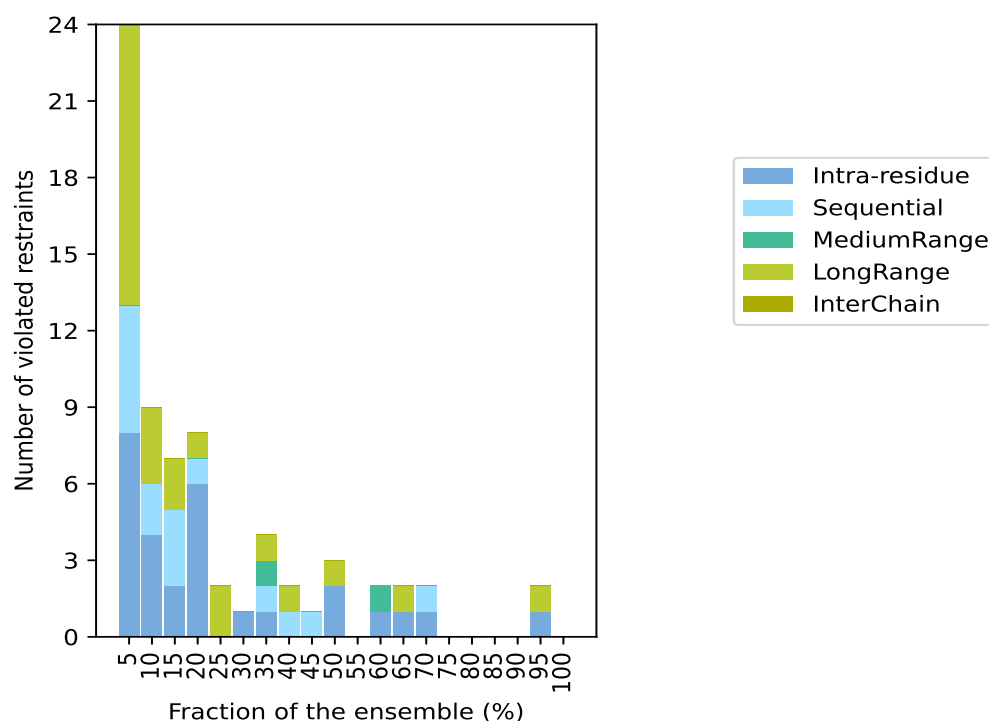
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 521(IR:237, SQ:135, MR:52, LR:97, IC:0) restraints are not 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>       | %     |
| 8                             | 5               | 0               | 11              | 0               | 24    | 1                        | 5.0   |
| 4                             | 2               | 0               | 3               | 0               | 9     | 2                        | 10.0  |
| 2                             | 3               | 0               | 2               | 0               | 7     | 3                        | 15.0  |
| 6                             | 1               | 0               | 1               | 0               | 8     | 4                        | 20.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 5                        | 25.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 6                        | 30.0  |
| 1                             | 1               | 1               | 1               | 0               | 4     | 7                        | 35.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 8                        | 40.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 9                        | 45.0  |
| 2                             | 0               | 0               | 1               | 0               | 3     | 10                       | 50.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 55.0  |
| 1                             | 0               | 1               | 0               | 0               | 2     | 12                       | 60.0  |
| 1                             | 0               | 0               | 1               | 0               | 2     | 13                       | 65.0  |
| 1                             | 1               | 0               | 0               | 0               | 2     | 14                       | 70.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 15                       | 75.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 16                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 85.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 18                       | 90.0  |
| 1                             | 0               | 0               | 1               | 0               | 2     | 19                       | 95.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 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

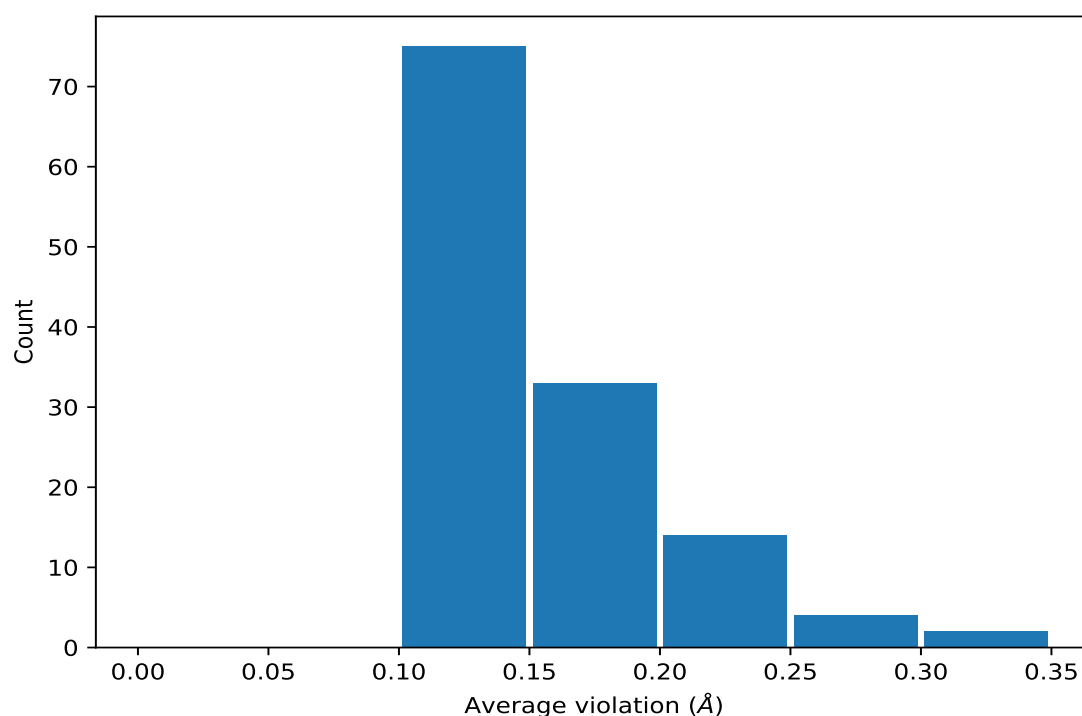
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 19                  | 0.19     | 0.06                | 0.18       |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 19                  | 0.19     | 0.06                | 0.18       |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 19                  | 0.19     | 0.06                | 0.18       |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 19                  | 0.19     | 0.06                | 0.18       |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 19                  | 0.19     | 0.06                | 0.18       |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 19                  | 0.19     | 0.06                | 0.18       |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 19                  | 0.19     | 0.06                | 0.18       |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 19                  | 0.19     | 0.06                | 0.18       |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 19                  | 0.19     | 0.06                | 0.18       |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 19                  | 0.19     | 0.06                | 0.18       |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 19                  | 0.19     | 0.06                | 0.18       |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 19                  | 0.19     | 0.06                | 0.18       |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2 | 19                  | 0.16     | 0.06                | 0.14       |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3 | 19                  | 0.16     | 0.06                | 0.14       |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD2 | 14                  | 0.24     | 0.06                | 0.24       |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD3 | 14                  | 0.24     | 0.06                | 0.24       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H    | 14                  | 0.13     | 0.02                | 0.12       |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG2  | 13                  | 0.19     | 0.02                | 0.19       |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG3  | 13                  | 0.19     | 0.02                | 0.19       |
| (1,97)  | 1:19:A:ALA:H    | 1:63:A:LEU:HG   | 13                  | 0.13     | 0.02                | 0.12       |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD2  | 12                  | 0.25     | 0.06                | 0.26       |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD3  | 12                  | 0.25     | 0.06                | 0.26       |
| (1,255) | 1:31:A:SER:H    | 1:34:A:CYS:H    | 12                  | 0.14     | 0.03                | 0.12       |
| (1,45)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HE2  | 10                  | 0.23     | 0.04                | 0.22       |
| (1,45)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HE3  | 10                  | 0.23     | 0.04                | 0.22       |
| (1,45)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HE2  | 10                  | 0.23     | 0.04                | 0.22       |
| (1,45)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HE3  | 10                  | 0.23     | 0.04                | 0.22       |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE2  | 10                  | 0.23     | 0.04                | 0.22       |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE3  | 10                  | 0.23     | 0.04                | 0.22       |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB1  | 10                  | 0.12     | 0.01                | 0.12       |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB2  | 10                  | 0.12     | 0.01                | 0.12       |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB3  | 10                  | 0.12     | 0.01                | 0.12       |
| (1,16)  | 1:8:A:CYS:HA    | 1:9:A:CYS:H     | 9                   | 0.21     | 0.06                | 0.24       |
| (1,383) | 1:45:A:LYS:HB2  | 1:46:A:ARG:H    | 8                   | 0.15     | 0.03                | 0.14       |
| (1,300) | 1:39:A:ILE:HD11 | 1:64:A:MET:H    | 8                   | 0.12     | 0.01                | 0.12       |
| (1,300) | 1:39:A:ILE:HD12 | 1:64:A:MET:H    | 8                   | 0.12     | 0.01                | 0.12       |
| (1,300) | 1:39:A:ILE:HD13 | 1:64:A:MET:H    | 8                   | 0.12     | 0.01                | 0.12       |
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE2  | 7                   | 0.2      | 0.05                | 0.23       |
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE3  | 7                   | 0.2      | 0.05                | 0.23       |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE2  | 7                   | 0.2      | 0.05                | 0.23       |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE3  | 7                   | 0.2      | 0.05                | 0.23       |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB1  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB2  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB3  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,121) | 1:20:A:LYS:HG2  | 1:21:A:VAL:H    | 7                   | 0.12     | 0.02                | 0.12       |
| (1,121) | 1:20:A:LYS:HG3  | 1:21:A:VAL:H    | 7                   | 0.12     | 0.02                | 0.12       |
| (1,568) | 1:67:A:LEU:HA   | 1:69:A:LYS:H    | 7                   | 0.12     | 0.01                | 0.11       |
| (1,377) | 1:45:A:LYS:HA   | 1:45:A:LYS:HB2  | 6                   | 0.21     | 0.01                | 0.21       |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB1  | 5                   | 0.14     | 0.02                | 0.14       |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB2  | 5                   | 0.14     | 0.02                | 0.14       |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB3  | 5                   | 0.14     | 0.02                | 0.14       |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB1  | 5                   | 0.14     | 0.02                | 0.14       |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB2  | 5                   | 0.14     | 0.02                | 0.14       |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB3  | 5                   | 0.14     | 0.02                | 0.14       |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD11 | 5                   | 0.12     | 0.02                | 0.11       |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD12 | 5                   | 0.12     | 0.02                | 0.11       |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD13 | 5                   | 0.12     | 0.02                | 0.11       |
| (1,583) | 1:69:A:LYS:HA   | 1:69:A:LYS:HE2  | 4                   | 0.16     | 0.07                | 0.14       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,583) | 1:69:A:LYS:HA   | 1:69:A:LYS:HE3  | 4                   | 0.16     | 0.07                | 0.14       |
| (1,81)  | 1:16:A:LYS:HB2  | 1:16:A:LYS:HD2  | 4                   | 0.15     | 0.03                | 0.15       |
| (1,81)  | 1:16:A:LYS:HB2  | 1:16:A:LYS:HD3  | 4                   | 0.15     | 0.03                | 0.15       |
| (1,81)  | 1:16:A:LYS:HB3  | 1:16:A:LYS:HD2  | 4                   | 0.15     | 0.03                | 0.15       |
| (1,81)  | 1:16:A:LYS:HB3  | 1:16:A:LYS:HD3  | 4                   | 0.15     | 0.03                | 0.15       |
| (1,133) | 1:22:A:VAL:HB   | 1:23:A:ARG:H    | 4                   | 0.15     | 0.0                 | 0.15       |
| (1,447) | 1:56:A:LYS:H    | 1:56:A:LYS:HG2  | 4                   | 0.14     | 0.06                | 0.11       |
| (1,447) | 1:56:A:LYS:H    | 1:56:A:LYS:HG3  | 4                   | 0.14     | 0.06                | 0.11       |
| (1,389) | 1:46:A:ARG:HA   | 1:46:A:ARG:HD2  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,389) | 1:46:A:ARG:HA   | 1:46:A:ARG:HD3  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,44)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HD2  | 4                   | 0.13     | 0.02                | 0.14       |
| (1,44)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HD3  | 4                   | 0.13     | 0.02                | 0.14       |
| (1,44)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HD2  | 4                   | 0.13     | 0.02                | 0.14       |
| (1,44)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HD3  | 4                   | 0.13     | 0.02                | 0.14       |
| (1,69)  | 1:15:A:ARG:HA   | 1:15:A:ARG:HD2  | 4                   | 0.13     | 0.02                | 0.12       |
| (1,69)  | 1:15:A:ARG:HA   | 1:15:A:ARG:HD3  | 4                   | 0.13     | 0.02                | 0.12       |
| (1,251) | 1:30:A:PRO:HG3  | 1:38:A:ALA:H    | 4                   | 0.11     | 0.01                | 0.12       |
| (1,118) | 1:20:A:LYS:HD2  | 1:21:A:VAL:H    | 3                   | 0.25     | 0.03                | 0.23       |
| (1,118) | 1:20:A:LYS:HD3  | 1:21:A:VAL:H    | 3                   | 0.25     | 0.03                | 0.23       |
| (1,587) | 1:69:A:LYS:HB2  | 1:70:A:THR:H    | 3                   | 0.16     | 0.05                | 0.13       |
| (1,587) | 1:69:A:LYS:HB3  | 1:70:A:THR:H    | 3                   | 0.16     | 0.05                | 0.13       |
| (1,183) | 1:25:A:TYR:HD1  | 1:63:A:LEU:HB2  | 3                   | 0.13     | 0.01                | 0.14       |
| (1,183) | 1:25:A:TYR:HD1  | 1:63:A:LEU:HB3  | 3                   | 0.13     | 0.01                | 0.14       |
| (1,183) | 1:25:A:TYR:HD2  | 1:63:A:LEU:HB2  | 3                   | 0.13     | 0.01                | 0.14       |
| (1,183) | 1:25:A:TYR:HD2  | 1:63:A:LEU:HB3  | 3                   | 0.13     | 0.01                | 0.14       |
| (1,580) | 1:69:A:LYS:H    | 1:69:A:LYS:HD2  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,580) | 1:69:A:LYS:H    | 1:69:A:LYS:HD3  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,200) | 1:26:A:ARG:H    | 1:40:A:LEU:HD11 | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,200) | 1:26:A:ARG:H    | 1:40:A:LEU:HD12 | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,200) | 1:26:A:ARG:H    | 1:40:A:LEU:HD13 | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,200) | 1:26:A:ARG:H    | 1:40:A:LEU:HD21 | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,200) | 1:26:A:ARG:H    | 1:40:A:LEU:HD22 | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,200) | 1:26:A:ARG:H    | 1:40:A:LEU:HD23 | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,513) | 1:61:A:GLN:H    | 1:61:A:GLN:HG2  | 3                   | 0.12     | 0.01                | 0.12       |
| (1,513) | 1:61:A:GLN:H    | 1:61:A:GLN:HG3  | 3                   | 0.12     | 0.01                | 0.12       |
| (1,280) | 1:37:A:PRO:HG2  | 1:38:A:ALA:H    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,280) | 1:37:A:PRO:HG3  | 1:38:A:ALA:H    | 3                   | 0.11     | 0.01                | 0.11       |
| (1,367) | 1:44:A:ARG:HA   | 1:44:A:ARG:HD2  | 2                   | 0.3      | 0.02                | 0.3        |
| (1,367) | 1:44:A:ARG:HA   | 1:44:A:ARG:HD3  | 2                   | 0.3      | 0.02                | 0.3        |
| (1,424) | 1:51:A:LEU:HG   | 1:52:A:CYS:H    | 2                   | 0.18     | 0.04                | 0.18       |
| (1,36)  | 1:10:A:LEU:HD11 | 1:50:A:GLU:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,36)  | 1:10:A:LEU:HD12 | 1:50:A:GLU:H    | 2                   | 0.16     | 0.01                | 0.16       |

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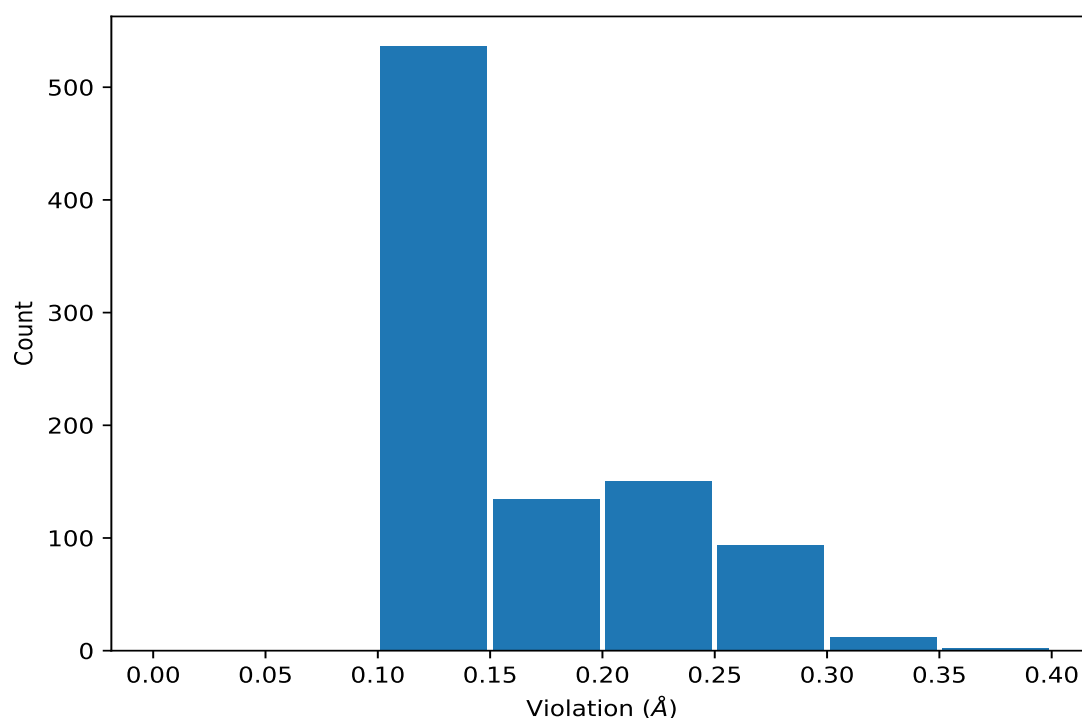
| Key     | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,36)  | 1:10:A:LEU:HD13 | 1:50:A:GLU:H   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,36)  | 1:10:A:LEU:HD21 | 1:50:A:GLU:H   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,36)  | 1:10:A:LEU:HD22 | 1:50:A:GLU:H   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,36)  | 1:10:A:LEU:HD23 | 1:50:A:GLU:H   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,204) | 1:26:A:ARG:HA   | 1:26:A:ARG:HD2 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,204) | 1:26:A:ARG:HA   | 1:26:A:ARG:HD3 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,323) | 1:40:A:LEU:HD21 | 1:52:A:CYS:H   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,323) | 1:40:A:LEU:HD22 | 1:52:A:CYS:H   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,323) | 1:40:A:LEU:HD23 | 1:52:A:CYS:H   | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,37)  | 1:10:A:LEU:HD11 | 1:50:A:GLU:HB2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,37)  | 1:10:A:LEU:HD11 | 1:50:A:GLU:HB3 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,37)  | 1:10:A:LEU:HD12 | 1:50:A:GLU:HB2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,37)  | 1:10:A:LEU:HD12 | 1:50:A:GLU:HB3 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,37)  | 1:10:A:LEU:HD13 | 1:50:A:GLU:HB2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,37)  | 1:10:A:LEU:HD13 | 1:50:A:GLU:HB3 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,37)  | 1:10:A:LEU:HD21 | 1:50:A:GLU:HB2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,37)  | 1:10:A:LEU:HD21 | 1:50:A:GLU:HB3 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,37)  | 1:10:A:LEU:HD22 | 1:50:A:GLU:HB2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,37)  | 1:10:A:LEU:HD22 | 1:50:A:GLU:HB3 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,37)  | 1:10:A:LEU:HD23 | 1:50:A:GLU:HB2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,37)  | 1:10:A:LEU:HD23 | 1:50:A:GLU:HB3 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,449) | 1:56:A:LYS:HA   | 1:56:A:LYS:HD2 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,449) | 1:56:A:LYS:HA   | 1:56:A:LYS:HD3 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,297) | 1:39:A:ILE:HD11 | 1:40:A:LEU:H   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,297) | 1:39:A:ILE:HD12 | 1:40:A:LEU:H   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,297) | 1:39:A:ILE:HD13 | 1:40:A:LEU:H   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,214) | 1:27:A:LYS:H    | 1:27:A:LYS:HD2 | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,214) | 1:27:A:LYS:H    | 1:27:A:LYS:HD3 | 2                   | 0.1      | 0.0                 | 0.1        |

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

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

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

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



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

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

| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,376) | 1:45:A:LYS:H   | 1:45:A:LYS:HD2 | 19       | 0.4           |
| (1,376) | 1:45:A:LYS:H   | 1:45:A:LYS:HD3 | 19       | 0.4           |
| (1,45)  | 1:11:A:LYS:HB2 | 1:11:A:LYS:HE2 | 19       | 0.34          |
| (1,45)  | 1:11:A:LYS:HB2 | 1:11:A:LYS:HE3 | 19       | 0.34          |
| (1,45)  | 1:11:A:LYS:HB3 | 1:11:A:LYS:HE2 | 19       | 0.34          |
| (1,45)  | 1:11:A:LYS:HB3 | 1:11:A:LYS:HE3 | 19       | 0.34          |
| (1,367) | 1:44:A:ARG:HA  | 1:44:A:ARG:HD2 | 19       | 0.32          |
| (1,367) | 1:44:A:ARG:HA  | 1:44:A:ARG:HD3 | 19       | 0.32          |
| (1,39)  | 1:11:A:LYS:H   | 1:11:A:LYS:HD2 | 16       | 0.32          |
| (1,39)  | 1:11:A:LYS:H   | 1:11:A:LYS:HD3 | 16       | 0.32          |
| (1,376) | 1:45:A:LYS:H   | 1:45:A:LYS:HD2 | 12       | 0.31          |
| (1,376) | 1:45:A:LYS:H   | 1:45:A:LYS:HD3 | 12       | 0.31          |
| (1,39)  | 1:11:A:LYS:H   | 1:11:A:LYS:HD2 | 6        | 0.31          |
| (1,39)  | 1:11:A:LYS:H   | 1:11:A:LYS:HD3 | 6        | 0.31          |
| (1,227) | 1:27:A:LYS:HB2 | 1:27:A:LYS:HE2 | 17       | 0.3           |
| (1,227) | 1:27:A:LYS:HB2 | 1:27:A:LYS:HE3 | 17       | 0.3           |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,227) | 1:27:A:LYS:HB3  | 1:27:A:LYS:HE2 | 17       | 0.3           |
| (1,227) | 1:27:A:LYS:HB3  | 1:27:A:LYS:HE3 | 17       | 0.3           |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD2 | 2        | 0.3           |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD3 | 2        | 0.3           |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD2 | 3        | 0.3           |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD3 | 3        | 0.3           |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 4        | 0.3           |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 4        | 0.3           |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 4        | 0.3           |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 4        | 0.3           |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 4        | 0.3           |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 4        | 0.3           |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 4        | 0.3           |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 4        | 0.3           |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 4        | 0.3           |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 4        | 0.3           |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 4        | 0.3           |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 4        | 0.3           |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 18       | 0.3           |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 18       | 0.3           |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 18       | 0.3           |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 18       | 0.3           |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 18       | 0.3           |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 18       | 0.3           |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 18       | 0.3           |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 18       | 0.3           |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 18       | 0.3           |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 18       | 0.3           |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 18       | 0.3           |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 18       | 0.3           |
| (1,16)  | 1:8:A:CYS:HA    | 1:9:A:CYS:H    | 6        | 0.3           |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD2 | 5        | 0.29          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD3 | 5        | 0.29          |
| (1,367) | 1:44:A:ARG:HA   | 1:44:A:ARG:HD2 | 6        | 0.29          |
| (1,367) | 1:44:A:ARG:HA   | 1:44:A:ARG:HD3 | 6        | 0.29          |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE2 | 12       | 0.29          |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE3 | 12       | 0.29          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2 | 9        | 0.29          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3 | 9        | 0.29          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2 | 13       | 0.29          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3 | 13       | 0.29          |
| (1,118) | 1:20:A:LYS:HD2  | 1:21:A:VAL:H   | 10       | 0.29          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,118) | 1:20:A:LYS:HD3  | 1:21:A:VAL:H   | 10       | 0.29          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 16       | 0.29          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 16       | 0.29          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 16       | 0.29          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 16       | 0.29          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 16       | 0.29          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 16       | 0.29          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 16       | 0.29          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 16       | 0.29          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 16       | 0.29          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 16       | 0.29          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 16       | 0.29          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 16       | 0.29          |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE2 | 18       | 0.28          |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE3 | 18       | 0.28          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2 | 20       | 0.28          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3 | 20       | 0.28          |
| (1,16)  | 1:8:A:CYS:HA    | 1:9:A:CYS:H    | 10       | 0.28          |
| (1,583) | 1:69:A:LYS:HA   | 1:69:A:LYS:HE2 | 16       | 0.27          |
| (1,583) | 1:69:A:LYS:HA   | 1:69:A:LYS:HE3 | 16       | 0.27          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD2 | 8        | 0.27          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD3 | 8        | 0.27          |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE2 | 13       | 0.27          |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE3 | 13       | 0.27          |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD2 | 9        | 0.27          |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD3 | 9        | 0.27          |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD2 | 11       | 0.27          |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD3 | 11       | 0.27          |
| (1,16)  | 1:8:A:CYS:HA    | 1:9:A:CYS:H    | 7        | 0.27          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD2 | 15       | 0.26          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD3 | 15       | 0.26          |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD2 | 1        | 0.26          |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD3 | 1        | 0.26          |
| (1,16)  | 1:8:A:CYS:HA    | 1:9:A:CYS:H    | 17       | 0.26          |
| (1,542) | 1:64:A:MET:H    | 1:64:A:MET:HG2 | 2        | 0.25          |
| (1,542) | 1:64:A:MET:H    | 1:64:A:MET:HG3 | 2        | 0.25          |
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE2 | 1        | 0.25          |
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE3 | 1        | 0.25          |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE2 | 1        | 0.25          |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE3 | 1        | 0.25          |
| (1,447) | 1:56:A:LYS:H    | 1:56:A:LYS:HG2 | 7        | 0.25          |
| (1,447) | 1:56:A:LYS:H    | 1:56:A:LYS:HG3 | 7        | 0.25          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD2 | 1        | 0.25          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD3 | 1        | 0.25          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD2 | 10       | 0.25          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD3 | 10       | 0.25          |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD2 | 4        | 0.25          |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD3 | 4        | 0.25          |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD2 | 5        | 0.25          |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD3 | 5        | 0.25          |
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE2 | 2        | 0.24          |
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE3 | 2        | 0.24          |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE2 | 2        | 0.24          |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE3 | 2        | 0.24          |
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE2 | 15       | 0.24          |
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE3 | 15       | 0.24          |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE2 | 15       | 0.24          |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE3 | 15       | 0.24          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD2 | 14       | 0.24          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD3 | 14       | 0.24          |
| (1,348) | 1:41:A:PHE:HE1  | 1:63:A:LEU:HG  | 18       | 0.24          |
| (1,78)  | 1:16:A:LYS:HA   | 1:16:A:LYS:HD2 | 17       | 0.24          |
| (1,78)  | 1:16:A:LYS:HA   | 1:16:A:LYS:HD3 | 17       | 0.24          |
| (1,45)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HE2 | 13       | 0.24          |
| (1,45)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HE3 | 13       | 0.24          |
| (1,45)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HE2 | 13       | 0.24          |
| (1,45)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HE3 | 13       | 0.24          |
| (1,45)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HE2 | 18       | 0.24          |
| (1,45)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HE3 | 18       | 0.24          |
| (1,45)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HE2 | 18       | 0.24          |
| (1,45)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HE3 | 18       | 0.24          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 14       | 0.24          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 14       | 0.24          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 14       | 0.24          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 14       | 0.24          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 14       | 0.24          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 14       | 0.24          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 14       | 0.24          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 14       | 0.24          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 14       | 0.24          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 14       | 0.24          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 14       | 0.24          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 14       | 0.24          |
| (1,16)  | 1:8:A:CYS:HA    | 1:9:A:CYS:H    | 14       | 0.24          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,587) | 1:69:A:LYS:HB2 | 1:70:A:THR:H   | 14       | 0.23          |
| (1,587) | 1:69:A:LYS:HB3 | 1:70:A:THR:H   | 14       | 0.23          |
| (1,453) | 1:56:A:LYS:HB2 | 1:56:A:LYS:HE2 | 16       | 0.23          |
| (1,453) | 1:56:A:LYS:HB2 | 1:56:A:LYS:HE3 | 16       | 0.23          |
| (1,453) | 1:56:A:LYS:HB3 | 1:56:A:LYS:HE2 | 16       | 0.23          |
| (1,453) | 1:56:A:LYS:HB3 | 1:56:A:LYS:HE3 | 16       | 0.23          |
| (1,377) | 1:45:A:LYS:HA  | 1:45:A:LYS:HB2 | 20       | 0.23          |
| (1,218) | 1:27:A:LYS:HA  | 1:27:A:LYS:HE2 | 1        | 0.23          |
| (1,218) | 1:27:A:LYS:HA  | 1:27:A:LYS:HE3 | 1        | 0.23          |
| (1,218) | 1:27:A:LYS:HA  | 1:27:A:LYS:HE2 | 11       | 0.23          |
| (1,218) | 1:27:A:LYS:HA  | 1:27:A:LYS:HE3 | 11       | 0.23          |
| (1,118) | 1:20:A:LYS:HD2 | 1:21:A:VAL:H   | 7        | 0.23          |
| (1,118) | 1:20:A:LYS:HD3 | 1:21:A:VAL:H   | 7        | 0.23          |
| (1,45)  | 1:11:A:LYS:HB2 | 1:11:A:LYS:HE2 | 17       | 0.23          |
| (1,45)  | 1:11:A:LYS:HB2 | 1:11:A:LYS:HE3 | 17       | 0.23          |
| (1,45)  | 1:11:A:LYS:HB3 | 1:11:A:LYS:HE2 | 17       | 0.23          |
| (1,45)  | 1:11:A:LYS:HB3 | 1:11:A:LYS:HE3 | 17       | 0.23          |
| (1,39)  | 1:11:A:LYS:H   | 1:11:A:LYS:HD2 | 19       | 0.23          |
| (1,39)  | 1:11:A:LYS:H   | 1:11:A:LYS:HD3 | 19       | 0.23          |
| (1,424) | 1:51:A:LEU:HG  | 1:52:A:CYS:H   | 6        | 0.22          |
| (1,377) | 1:45:A:LYS:HA  | 1:45:A:LYS:HB2 | 3        | 0.22          |
| (1,218) | 1:27:A:LYS:HA  | 1:27:A:LYS:HE2 | 4        | 0.22          |
| (1,218) | 1:27:A:LYS:HA  | 1:27:A:LYS:HE3 | 4        | 0.22          |
| (1,149) | 1:23:A:ARG:H   | 1:23:A:ARG:HG2 | 18       | 0.22          |
| (1,149) | 1:23:A:ARG:H   | 1:23:A:ARG:HG3 | 18       | 0.22          |
| (1,118) | 1:20:A:LYS:HD2 | 1:21:A:VAL:H   | 5        | 0.22          |
| (1,118) | 1:20:A:LYS:HD3 | 1:21:A:VAL:H   | 5        | 0.22          |
| (1,45)  | 1:11:A:LYS:HB2 | 1:11:A:LYS:HE2 | 4        | 0.22          |
| (1,45)  | 1:11:A:LYS:HB2 | 1:11:A:LYS:HE3 | 4        | 0.22          |
| (1,45)  | 1:11:A:LYS:HB3 | 1:11:A:LYS:HE2 | 4        | 0.22          |
| (1,45)  | 1:11:A:LYS:HB3 | 1:11:A:LYS:HE3 | 4        | 0.22          |
| (1,45)  | 1:11:A:LYS:HB2 | 1:11:A:LYS:HE2 | 7        | 0.22          |
| (1,45)  | 1:11:A:LYS:HB2 | 1:11:A:LYS:HE3 | 7        | 0.22          |
| (1,45)  | 1:11:A:LYS:HB3 | 1:11:A:LYS:HE2 | 7        | 0.22          |
| (1,45)  | 1:11:A:LYS:HB3 | 1:11:A:LYS:HE3 | 7        | 0.22          |
| (1,45)  | 1:11:A:LYS:HB2 | 1:11:A:LYS:HE2 | 8        | 0.22          |
| (1,45)  | 1:11:A:LYS:HB2 | 1:11:A:LYS:HE3 | 8        | 0.22          |
| (1,45)  | 1:11:A:LYS:HB3 | 1:11:A:LYS:HE2 | 8        | 0.22          |
| (1,45)  | 1:11:A:LYS:HB3 | 1:11:A:LYS:HE3 | 8        | 0.22          |
| (1,45)  | 1:11:A:LYS:HB2 | 1:11:A:LYS:HE2 | 20       | 0.22          |
| (1,45)  | 1:11:A:LYS:HB2 | 1:11:A:LYS:HE3 | 20       | 0.22          |
| (1,45)  | 1:11:A:LYS:HB3 | 1:11:A:LYS:HE2 | 20       | 0.22          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,45)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HE3 | 20       | 0.22          |
| (1,377) | 1:45:A:LYS:HA   | 1:45:A:LYS:HB2 | 13       | 0.21          |
| (1,377) | 1:45:A:LYS:HA   | 1:45:A:LYS:HB2 | 18       | 0.21          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG2 | 11       | 0.21          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG3 | 11       | 0.21          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG2 | 17       | 0.21          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG3 | 17       | 0.21          |
| (1,45)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HE2 | 11       | 0.21          |
| (1,45)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HE3 | 11       | 0.21          |
| (1,45)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HE2 | 11       | 0.21          |
| (1,45)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HE3 | 11       | 0.21          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 3        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 3        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 3        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 3        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 3        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 3        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 3        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 3        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 3        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 3        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 3        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 3        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 9        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 9        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 9        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 9        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 9        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 9        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 9        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 9        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 9        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 9        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 9        | 0.21          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 9        | 0.21          |
| (1,383) | 1:45:A:LYS:HB2  | 1:46:A:ARG:H   | 12       | 0.2           |
| (1,377) | 1:45:A:LYS:HA   | 1:45:A:LYS:HB2 | 4        | 0.2           |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD2 | 2        | 0.2           |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD3 | 2        | 0.2           |
| (1,255) | 1:31:A:SER:H    | 1:34:A:CYS:H   | 8        | 0.2           |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE2 | 8        | 0.2           |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE3 | 8        | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG2  | 1        | 0.2           |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG3  | 1        | 0.2           |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG2  | 5        | 0.2           |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG3  | 5        | 0.2           |
| (1,45)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HE2  | 1        | 0.2           |
| (1,45)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HE3  | 1        | 0.2           |
| (1,45)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HE2  | 1        | 0.2           |
| (1,45)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HE3  | 1        | 0.2           |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2  | 1        | 0.2           |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3  | 1        | 0.2           |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2  | 1        | 0.2           |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3  | 1        | 0.2           |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2  | 1        | 0.2           |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3  | 1        | 0.2           |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2  | 1        | 0.2           |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3  | 1        | 0.2           |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2  | 1        | 0.2           |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3  | 1        | 0.2           |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2  | 1        | 0.2           |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3  | 1        | 0.2           |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2  | 20       | 0.2           |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3  | 20       | 0.2           |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2  | 20       | 0.2           |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3  | 20       | 0.2           |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2  | 20       | 0.2           |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3  | 20       | 0.2           |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2  | 20       | 0.2           |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3  | 20       | 0.2           |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2  | 20       | 0.2           |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3  | 20       | 0.2           |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2  | 20       | 0.2           |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3  | 20       | 0.2           |
| (1,383) | 1:45:A:LYS:HB2  | 1:46:A:ARG:H    | 10       | 0.19          |
| (1,377) | 1:45:A:LYS:HA   | 1:45:A:LYS:HB2  | 6        | 0.19          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD2  | 7        | 0.19          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD3  | 7        | 0.19          |
| (1,209) | 1:26:A:ARG:HB2  | 1:40:A:LEU:HD11 | 5        | 0.19          |
| (1,209) | 1:26:A:ARG:HB2  | 1:40:A:LEU:HD12 | 5        | 0.19          |
| (1,209) | 1:26:A:ARG:HB2  | 1:40:A:LEU:HD13 | 5        | 0.19          |
| (1,209) | 1:26:A:ARG:HB2  | 1:40:A:LEU:HD21 | 5        | 0.19          |
| (1,209) | 1:26:A:ARG:HB2  | 1:40:A:LEU:HD22 | 5        | 0.19          |
| (1,209) | 1:26:A:ARG:HB2  | 1:40:A:LEU:HD23 | 5        | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,209) | 1:26:A:ARG:HB3  | 1:40:A:LEU:HD11 | 5        | 0.19          |
| (1,209) | 1:26:A:ARG:HB3  | 1:40:A:LEU:HD12 | 5        | 0.19          |
| (1,209) | 1:26:A:ARG:HB3  | 1:40:A:LEU:HD13 | 5        | 0.19          |
| (1,209) | 1:26:A:ARG:HB3  | 1:40:A:LEU:HD21 | 5        | 0.19          |
| (1,209) | 1:26:A:ARG:HB3  | 1:40:A:LEU:HD22 | 5        | 0.19          |
| (1,209) | 1:26:A:ARG:HB3  | 1:40:A:LEU:HD23 | 5        | 0.19          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG2  | 3        | 0.19          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG3  | 3        | 0.19          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG2  | 7        | 0.19          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG3  | 7        | 0.19          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG2  | 19       | 0.19          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG3  | 19       | 0.19          |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD2  | 12       | 0.19          |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD3  | 12       | 0.19          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2  | 2        | 0.19          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3  | 2        | 0.19          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2  | 2        | 0.19          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3  | 2        | 0.19          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2  | 2        | 0.19          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3  | 2        | 0.19          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2  | 2        | 0.19          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3  | 2        | 0.19          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2  | 2        | 0.19          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3  | 2        | 0.19          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2  | 2        | 0.19          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3  | 2        | 0.19          |
| (1,383) | 1:45:A:LYS:HB2  | 1:46:A:ARG:H    | 19       | 0.18          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD2  | 9        | 0.18          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD3  | 9        | 0.18          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD2  | 16       | 0.18          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD3  | 16       | 0.18          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD2  | 17       | 0.18          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD3  | 17       | 0.18          |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE2  | 6        | 0.18          |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE3  | 6        | 0.18          |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE2  | 19       | 0.18          |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE3  | 19       | 0.18          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2  | 4        | 0.18          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3  | 4        | 0.18          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG2  | 2        | 0.18          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG3  | 2        | 0.18          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG2  | 4        | 0.18          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG3 | 4        | 0.18          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG2 | 8        | 0.18          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG3 | 8        | 0.18          |
| (1,81)  | 1:16:A:LYS:HB2  | 1:16:A:LYS:HD2 | 18       | 0.18          |
| (1,81)  | 1:16:A:LYS:HB2  | 1:16:A:LYS:HD3 | 18       | 0.18          |
| (1,81)  | 1:16:A:LYS:HB3  | 1:16:A:LYS:HD2 | 18       | 0.18          |
| (1,81)  | 1:16:A:LYS:HB3  | 1:16:A:LYS:HD3 | 18       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 10       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 10       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 10       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 10       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 10       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 10       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 10       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 10       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 10       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 10       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 10       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 10       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 17       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 17       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 17       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 17       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 17       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 17       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 17       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 17       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 17       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 17       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 17       | 0.18          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 17       | 0.18          |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H   | 14       | 0.17          |
| (1,255) | 1:31:A:SER:H    | 1:34:A:CYS:H   | 9        | 0.17          |
| (1,255) | 1:31:A:SER:H    | 1:34:A:CYS:H   | 10       | 0.17          |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE2 | 7        | 0.17          |
| (1,218) | 1:27:A:LYS:HA   | 1:27:A:LYS:HE3 | 7        | 0.17          |
| (1,204) | 1:26:A:ARG:HA   | 1:26:A:ARG:HD2 | 5        | 0.17          |
| (1,204) | 1:26:A:ARG:HA   | 1:26:A:ARG:HD3 | 5        | 0.17          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2 | 3        | 0.17          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3 | 3        | 0.17          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG2 | 14       | 0.17          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG3 | 14       | 0.17          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,97)  | 1:19:A:ALA:H    | 1:63:A:LEU:HG  | 17       | 0.17          |
| (1,81)  | 1:16:A:LYS:HB2  | 1:16:A:LYS:HD2 | 10       | 0.17          |
| (1,81)  | 1:16:A:LYS:HB2  | 1:16:A:LYS:HD3 | 10       | 0.17          |
| (1,81)  | 1:16:A:LYS:HB3  | 1:16:A:LYS:HD2 | 10       | 0.17          |
| (1,81)  | 1:16:A:LYS:HB3  | 1:16:A:LYS:HD3 | 10       | 0.17          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 15       | 0.17          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 15       | 0.17          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 15       | 0.17          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 15       | 0.17          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 15       | 0.17          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 15       | 0.17          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 15       | 0.17          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 15       | 0.17          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 15       | 0.17          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 15       | 0.17          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 15       | 0.17          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 15       | 0.17          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB1 | 15       | 0.17          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB2 | 15       | 0.17          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB3 | 15       | 0.17          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB1 | 15       | 0.17          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB2 | 15       | 0.17          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB3 | 15       | 0.17          |
| (1,404) | 1:48:A:GLN:HB2  | 1:49:A:ALA:H   | 3        | 0.16          |
| (1,404) | 1:48:A:GLN:HB3  | 1:49:A:ALA:H   | 3        | 0.16          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2 | 7        | 0.16          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3 | 7        | 0.16          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2 | 8        | 0.16          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3 | 8        | 0.16          |
| (1,97)  | 1:19:A:ALA:H    | 1:63:A:LEU:HG  | 5        | 0.16          |
| (1,97)  | 1:19:A:ALA:H    | 1:63:A:LEU:HG  | 19       | 0.16          |
| (1,69)  | 1:15:A:ARG:HA   | 1:15:A:ARG:HD2 | 12       | 0.16          |
| (1,69)  | 1:15:A:ARG:HA   | 1:15:A:ARG:HD3 | 12       | 0.16          |
| (1,36)  | 1:10:A:LEU:HD11 | 1:50:A:GLU:H   | 20       | 0.16          |
| (1,36)  | 1:10:A:LEU:HD12 | 1:50:A:GLU:H   | 20       | 0.16          |
| (1,36)  | 1:10:A:LEU:HD13 | 1:50:A:GLU:H   | 20       | 0.16          |
| (1,36)  | 1:10:A:LEU:HD21 | 1:50:A:GLU:H   | 20       | 0.16          |
| (1,36)  | 1:10:A:LEU:HD22 | 1:50:A:GLU:H   | 20       | 0.16          |
| (1,36)  | 1:10:A:LEU:HD23 | 1:50:A:GLU:H   | 20       | 0.16          |
| (1,16)  | 1:8:A:CYS:HA    | 1:9:A:CYS:H    | 2        | 0.16          |
| (1,584) | 1:69:A:LYS:HB2  | 1:69:A:LYS:HD2 | 6        | 0.15          |
| (1,584) | 1:69:A:LYS:HB2  | 1:69:A:LYS:HD3 | 6        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,584) | 1:69:A:LYS:HB3  | 1:69:A:LYS:HD2  | 6        | 0.15          |
| (1,584) | 1:69:A:LYS:HB3  | 1:69:A:LYS:HD3  | 6        | 0.15          |
| (1,583) | 1:69:A:LYS:HA   | 1:69:A:LYS:HE2  | 9        | 0.15          |
| (1,583) | 1:69:A:LYS:HA   | 1:69:A:LYS:HE3  | 9        | 0.15          |
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE2  | 10       | 0.15          |
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE3  | 10       | 0.15          |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE2  | 10       | 0.15          |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE3  | 10       | 0.15          |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H    | 2        | 0.15          |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H    | 16       | 0.15          |
| (1,389) | 1:46:A:ARG:HA   | 1:46:A:ARG:HD2  | 17       | 0.15          |
| (1,389) | 1:46:A:ARG:HA   | 1:46:A:ARG:HD3  | 17       | 0.15          |
| (1,383) | 1:45:A:LYS:HB2  | 1:46:A:ARG:H    | 7        | 0.15          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD2  | 11       | 0.15          |
| (1,376) | 1:45:A:LYS:H    | 1:45:A:LYS:HD3  | 11       | 0.15          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB1  | 18       | 0.15          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB2  | 18       | 0.15          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB3  | 18       | 0.15          |
| (1,299) | 1:39:A:ILE:HD11 | 1:60:A:VAL:HG11 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD11 | 1:60:A:VAL:HG12 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD11 | 1:60:A:VAL:HG13 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD11 | 1:60:A:VAL:HG21 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD11 | 1:60:A:VAL:HG22 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD11 | 1:60:A:VAL:HG23 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD12 | 1:60:A:VAL:HG11 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD12 | 1:60:A:VAL:HG12 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD12 | 1:60:A:VAL:HG13 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD12 | 1:60:A:VAL:HG21 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD12 | 1:60:A:VAL:HG22 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD12 | 1:60:A:VAL:HG23 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD13 | 1:60:A:VAL:HG11 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD13 | 1:60:A:VAL:HG12 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD13 | 1:60:A:VAL:HG13 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD13 | 1:60:A:VAL:HG21 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD13 | 1:60:A:VAL:HG22 | 9        | 0.15          |
| (1,299) | 1:39:A:ILE:HD13 | 1:60:A:VAL:HG23 | 9        | 0.15          |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD11 | 6        | 0.15          |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD12 | 6        | 0.15          |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD13 | 6        | 0.15          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2  | 12       | 0.15          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3  | 12       | 0.15          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2  | 14       | 0.15          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3 | 14       | 0.15          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG2 | 15       | 0.15          |
| (1,149) | 1:23:A:ARG:H    | 1:23:A:ARG:HG3 | 15       | 0.15          |
| (1,133) | 1:22:A:VAL:HB   | 1:23:A:ARG:H   | 5        | 0.15          |
| (1,133) | 1:22:A:VAL:HB   | 1:23:A:ARG:H   | 11       | 0.15          |
| (1,121) | 1:20:A:LYS:HG2  | 1:21:A:VAL:H   | 14       | 0.15          |
| (1,121) | 1:20:A:LYS:HG3  | 1:21:A:VAL:H   | 14       | 0.15          |
| (1,44)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HD2 | 15       | 0.15          |
| (1,44)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HD3 | 15       | 0.15          |
| (1,44)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HD2 | 15       | 0.15          |
| (1,44)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HD3 | 15       | 0.15          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 6        | 0.15          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 6        | 0.15          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 6        | 0.15          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 6        | 0.15          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 6        | 0.15          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 6        | 0.15          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 6        | 0.15          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 6        | 0.15          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 6        | 0.15          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 6        | 0.15          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 6        | 0.15          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 6        | 0.15          |
| (1,36)  | 1:10:A:LEU:HD11 | 1:50:A:GLU:H   | 15       | 0.15          |
| (1,36)  | 1:10:A:LEU:HD12 | 1:50:A:GLU:H   | 15       | 0.15          |
| (1,36)  | 1:10:A:LEU:HD13 | 1:50:A:GLU:H   | 15       | 0.15          |
| (1,36)  | 1:10:A:LEU:HD21 | 1:50:A:GLU:H   | 15       | 0.15          |
| (1,36)  | 1:10:A:LEU:HD22 | 1:50:A:GLU:H   | 15       | 0.15          |
| (1,36)  | 1:10:A:LEU:HD23 | 1:50:A:GLU:H   | 15       | 0.15          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB1 | 14       | 0.15          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB2 | 14       | 0.15          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB3 | 14       | 0.15          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB1 | 14       | 0.15          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB2 | 14       | 0.15          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB3 | 14       | 0.15          |
| (1,16)  | 1:8:A:CYS:HA    | 1:9:A:CYS:H    | 8        | 0.15          |
| (1,16)  | 1:8:A:CYS:HA    | 1:9:A:CYS:H    | 19       | 0.15          |
| (1,7)   | 1:6:A:GLN:H     | 1:6:A:GLN:HG2  | 18       | 0.15          |
| (1,7)   | 1:6:A:GLN:H     | 1:6:A:GLN:HG3  | 18       | 0.15          |
| (1,580) | 1:69:A:LYS:H    | 1:69:A:LYS:HD2 | 14       | 0.14          |
| (1,580) | 1:69:A:LYS:H    | 1:69:A:LYS:HD3 | 14       | 0.14          |
| (1,568) | 1:67:A:LEU:HA   | 1:69:A:LYS:H   | 1        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE2  | 14       | 0.14          |
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE3  | 14       | 0.14          |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE2  | 14       | 0.14          |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE3  | 14       | 0.14          |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H    | 12       | 0.14          |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H    | 20       | 0.14          |
| (1,389) | 1:46:A:ARG:HA   | 1:46:A:ARG:HD2  | 6        | 0.14          |
| (1,389) | 1:46:A:ARG:HA   | 1:46:A:ARG:HD3  | 6        | 0.14          |
| (1,389) | 1:46:A:ARG:HA   | 1:46:A:ARG:HD2  | 13       | 0.14          |
| (1,389) | 1:46:A:ARG:HA   | 1:46:A:ARG:HD3  | 13       | 0.14          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB1  | 15       | 0.14          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB2  | 15       | 0.14          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB3  | 15       | 0.14          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB1  | 17       | 0.14          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB2  | 17       | 0.14          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB3  | 17       | 0.14          |
| (1,300) | 1:39:A:ILE:HD11 | 1:64:A:MET:H    | 19       | 0.14          |
| (1,300) | 1:39:A:ILE:HD12 | 1:64:A:MET:H    | 19       | 0.14          |
| (1,300) | 1:39:A:ILE:HD13 | 1:64:A:MET:H    | 19       | 0.14          |
| (1,255) | 1:31:A:SER:H    | 1:34:A:CYS:H    | 7        | 0.14          |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD11 | 1        | 0.14          |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD12 | 1        | 0.14          |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD13 | 1        | 0.14          |
| (1,183) | 1:25:A:TYR:HD1  | 1:63:A:LEU:HB2  | 13       | 0.14          |
| (1,183) | 1:25:A:TYR:HD1  | 1:63:A:LEU:HB3  | 13       | 0.14          |
| (1,183) | 1:25:A:TYR:HD2  | 1:63:A:LEU:HB2  | 13       | 0.14          |
| (1,183) | 1:25:A:TYR:HD2  | 1:63:A:LEU:HB3  | 13       | 0.14          |
| (1,183) | 1:25:A:TYR:HD1  | 1:63:A:LEU:HB2  | 20       | 0.14          |
| (1,183) | 1:25:A:TYR:HD1  | 1:63:A:LEU:HB3  | 20       | 0.14          |
| (1,183) | 1:25:A:TYR:HD2  | 1:63:A:LEU:HB2  | 20       | 0.14          |
| (1,183) | 1:25:A:TYR:HD2  | 1:63:A:LEU:HB3  | 20       | 0.14          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2  | 10       | 0.14          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3  | 10       | 0.14          |
| (1,133) | 1:22:A:VAL:HB   | 1:23:A:ARG:H    | 6        | 0.14          |
| (1,133) | 1:22:A:VAL:HB   | 1:23:A:ARG:H    | 18       | 0.14          |
| (1,44)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HD2  | 10       | 0.14          |
| (1,44)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HD3  | 10       | 0.14          |
| (1,44)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HD2  | 10       | 0.14          |
| (1,44)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HD3  | 10       | 0.14          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2  | 5        | 0.14          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3  | 5        | 0.14          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2  | 5        | 0.14          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 5        | 0.14          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 5        | 0.14          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 5        | 0.14          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 5        | 0.14          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 5        | 0.14          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 5        | 0.14          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 5        | 0.14          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 5        | 0.14          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 5        | 0.14          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 12       | 0.14          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 12       | 0.14          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 12       | 0.14          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 12       | 0.14          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 12       | 0.14          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 12       | 0.14          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 12       | 0.14          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 12       | 0.14          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 12       | 0.14          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 12       | 0.14          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 12       | 0.14          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 12       | 0.14          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB1 | 13       | 0.14          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB2 | 13       | 0.14          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB3 | 13       | 0.14          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB1 | 13       | 0.14          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB2 | 13       | 0.14          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB3 | 13       | 0.14          |
| (1,587) | 1:69:A:LYS:HB2  | 1:70:A:THR:H   | 9        | 0.13          |
| (1,587) | 1:69:A:LYS:HB3  | 1:70:A:THR:H   | 9        | 0.13          |
| (1,587) | 1:69:A:LYS:HB2  | 1:70:A:THR:H   | 18       | 0.13          |
| (1,587) | 1:69:A:LYS:HB3  | 1:70:A:THR:H   | 18       | 0.13          |
| (1,585) | 1:69:A:LYS:HB2  | 1:69:A:LYS:HE2 | 16       | 0.13          |
| (1,585) | 1:69:A:LYS:HB2  | 1:69:A:LYS:HE3 | 16       | 0.13          |
| (1,585) | 1:69:A:LYS:HB3  | 1:69:A:LYS:HE2 | 16       | 0.13          |
| (1,585) | 1:69:A:LYS:HB3  | 1:69:A:LYS:HE3 | 16       | 0.13          |
| (1,580) | 1:69:A:LYS:H    | 1:69:A:LYS:HD2 | 18       | 0.13          |
| (1,580) | 1:69:A:LYS:H    | 1:69:A:LYS:HD3 | 18       | 0.13          |
| (1,568) | 1:67:A:LEU:HA   | 1:69:A:LYS:H   | 2        | 0.13          |
| (1,513) | 1:61:A:GLN:H    | 1:61:A:GLN:HG2 | 3        | 0.13          |
| (1,513) | 1:61:A:GLN:H    | 1:61:A:GLN:HG3 | 3        | 0.13          |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H   | 9        | 0.13          |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H   | 10       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,424) | 1:51:A:LEU:HG   | 1:52:A:CYS:H    | 9        | 0.13          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB1  | 12       | 0.13          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB2  | 12       | 0.13          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB3  | 12       | 0.13          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB1  | 14       | 0.13          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB2  | 14       | 0.13          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB3  | 14       | 0.13          |
| (1,345) | 1:41:A:PHE:HD1  | 1:67:A:LEU:HD11 | 14       | 0.13          |
| (1,345) | 1:41:A:PHE:HD1  | 1:67:A:LEU:HD12 | 14       | 0.13          |
| (1,345) | 1:41:A:PHE:HD1  | 1:67:A:LEU:HD13 | 14       | 0.13          |
| (1,345) | 1:41:A:PHE:HD1  | 1:67:A:LEU:HD21 | 14       | 0.13          |
| (1,345) | 1:41:A:PHE:HD1  | 1:67:A:LEU:HD22 | 14       | 0.13          |
| (1,345) | 1:41:A:PHE:HD1  | 1:67:A:LEU:HD23 | 14       | 0.13          |
| (1,322) | 1:40:A:LEU:HD11 | 1:52:A:CYS:HA   | 2        | 0.13          |
| (1,322) | 1:40:A:LEU:HD12 | 1:52:A:CYS:HA   | 2        | 0.13          |
| (1,322) | 1:40:A:LEU:HD13 | 1:52:A:CYS:HA   | 2        | 0.13          |
| (1,300) | 1:39:A:ILE:HD11 | 1:64:A:MET:H    | 10       | 0.13          |
| (1,300) | 1:39:A:ILE:HD12 | 1:64:A:MET:H    | 10       | 0.13          |
| (1,300) | 1:39:A:ILE:HD13 | 1:64:A:MET:H    | 10       | 0.13          |
| (1,300) | 1:39:A:ILE:HD11 | 1:64:A:MET:H    | 12       | 0.13          |
| (1,300) | 1:39:A:ILE:HD12 | 1:64:A:MET:H    | 12       | 0.13          |
| (1,300) | 1:39:A:ILE:HD13 | 1:64:A:MET:H    | 12       | 0.13          |
| (1,255) | 1:31:A:SER:H    | 1:34:A:CYS:H    | 12       | 0.13          |
| (1,255) | 1:31:A:SER:H    | 1:34:A:CYS:H    | 20       | 0.13          |
| (1,234) | 1:28:A:GLN:H    | 1:40:A:LEU:HD11 | 16       | 0.13          |
| (1,234) | 1:28:A:GLN:H    | 1:40:A:LEU:HD12 | 16       | 0.13          |
| (1,234) | 1:28:A:GLN:H    | 1:40:A:LEU:HD13 | 16       | 0.13          |
| (1,234) | 1:28:A:GLN:H    | 1:40:A:LEU:HD21 | 16       | 0.13          |
| (1,234) | 1:28:A:GLN:H    | 1:40:A:LEU:HD22 | 16       | 0.13          |
| (1,234) | 1:28:A:GLN:H    | 1:40:A:LEU:HD23 | 16       | 0.13          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2  | 5        | 0.13          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3  | 5        | 0.13          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2  | 6        | 0.13          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3  | 6        | 0.13          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2  | 11       | 0.13          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3  | 11       | 0.13          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2  | 15       | 0.13          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3  | 15       | 0.13          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2  | 16       | 0.13          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3  | 16       | 0.13          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2  | 18       | 0.13          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3  | 18       | 0.13          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,121) | 1:20:A:LYS:HG2  | 1:21:A:VAL:H   | 9        | 0.13          |
| (1,121) | 1:20:A:LYS:HG3  | 1:21:A:VAL:H   | 9        | 0.13          |
| (1,97)  | 1:19:A:ALA:H    | 1:63:A:LEU:HG  | 2        | 0.13          |
| (1,97)  | 1:19:A:ALA:H    | 1:63:A:LEU:HG  | 9        | 0.13          |
| (1,81)  | 1:16:A:LYS:HB2  | 1:16:A:LYS:HD2 | 4        | 0.13          |
| (1,81)  | 1:16:A:LYS:HB2  | 1:16:A:LYS:HD3 | 4        | 0.13          |
| (1,81)  | 1:16:A:LYS:HB3  | 1:16:A:LYS:HD2 | 4        | 0.13          |
| (1,81)  | 1:16:A:LYS:HB3  | 1:16:A:LYS:HD3 | 4        | 0.13          |
| (1,44)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HD2 | 14       | 0.13          |
| (1,44)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HD3 | 14       | 0.13          |
| (1,44)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HD2 | 14       | 0.13          |
| (1,44)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HD3 | 14       | 0.13          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 11       | 0.13          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 11       | 0.13          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 11       | 0.13          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 11       | 0.13          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 11       | 0.13          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 11       | 0.13          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 11       | 0.13          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 11       | 0.13          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 11       | 0.13          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 11       | 0.13          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 11       | 0.13          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 11       | 0.13          |
| (1,583) | 1:69:A:LYS:HA   | 1:69:A:LYS:HE2 | 2        | 0.12          |
| (1,583) | 1:69:A:LYS:HA   | 1:69:A:LYS:HE3 | 2        | 0.12          |
| (1,580) | 1:69:A:LYS:H    | 1:69:A:LYS:HD2 | 9        | 0.12          |
| (1,580) | 1:69:A:LYS:H    | 1:69:A:LYS:HD3 | 9        | 0.12          |
| (1,568) | 1:67:A:LEU:HA   | 1:69:A:LYS:H   | 13       | 0.12          |
| (1,513) | 1:61:A:GLN:H    | 1:61:A:GLN:HG2 | 9        | 0.12          |
| (1,513) | 1:61:A:GLN:H    | 1:61:A:GLN:HG3 | 9        | 0.12          |
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE2 | 18       | 0.12          |
| (1,453) | 1:56:A:LYS:HB2  | 1:56:A:LYS:HE3 | 18       | 0.12          |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE2 | 18       | 0.12          |
| (1,453) | 1:56:A:LYS:HB3  | 1:56:A:LYS:HE3 | 18       | 0.12          |
| (1,449) | 1:56:A:LYS:HA   | 1:56:A:LYS:HD2 | 17       | 0.12          |
| (1,449) | 1:56:A:LYS:HA   | 1:56:A:LYS:HD3 | 17       | 0.12          |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H   | 1        | 0.12          |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H   | 11       | 0.12          |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H   | 15       | 0.12          |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H   | 19       | 0.12          |
| (1,418) | 1:51:A:LEU:H    | 1:51:A:LEU:HG  | 3        | 0.12          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,389) | 1:46:A:ARG:HA   | 1:46:A:ARG:HD2 | 3        | 0.12          |
| (1,389) | 1:46:A:ARG:HA   | 1:46:A:ARG:HD3 | 3        | 0.12          |
| (1,383) | 1:45:A:LYS:HB2  | 1:46:A:ARG:H   | 2        | 0.12          |
| (1,383) | 1:45:A:LYS:HB2  | 1:46:A:ARG:H   | 5        | 0.12          |
| (1,383) | 1:45:A:LYS:HB2  | 1:46:A:ARG:H   | 6        | 0.12          |
| (1,383) | 1:45:A:LYS:HB2  | 1:46:A:ARG:H   | 8        | 0.12          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB1 | 1        | 0.12          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB2 | 1        | 0.12          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB3 | 1        | 0.12          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB1 | 4        | 0.12          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB2 | 4        | 0.12          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB3 | 4        | 0.12          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB1 | 5        | 0.12          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB2 | 5        | 0.12          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB3 | 5        | 0.12          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB1 | 7        | 0.12          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB2 | 7        | 0.12          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB3 | 7        | 0.12          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB1 | 6        | 0.12          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB2 | 6        | 0.12          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB3 | 6        | 0.12          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB1 | 18       | 0.12          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB2 | 18       | 0.12          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB3 | 18       | 0.12          |
| (1,323) | 1:40:A:LEU:HD21 | 1:52:A:CYS:H   | 14       | 0.12          |
| (1,323) | 1:40:A:LEU:HD22 | 1:52:A:CYS:H   | 14       | 0.12          |
| (1,323) | 1:40:A:LEU:HD23 | 1:52:A:CYS:H   | 14       | 0.12          |
| (1,300) | 1:39:A:ILE:HD11 | 1:64:A:MET:H   | 2        | 0.12          |
| (1,300) | 1:39:A:ILE:HD12 | 1:64:A:MET:H   | 2        | 0.12          |
| (1,300) | 1:39:A:ILE:HD13 | 1:64:A:MET:H   | 2        | 0.12          |
| (1,300) | 1:39:A:ILE:HD11 | 1:64:A:MET:H   | 17       | 0.12          |
| (1,300) | 1:39:A:ILE:HD12 | 1:64:A:MET:H   | 17       | 0.12          |
| (1,300) | 1:39:A:ILE:HD13 | 1:64:A:MET:H   | 17       | 0.12          |
| (1,280) | 1:37:A:PRO:HG2  | 1:38:A:ALA:H   | 6        | 0.12          |
| (1,280) | 1:37:A:PRO:HG3  | 1:38:A:ALA:H   | 6        | 0.12          |
| (1,255) | 1:31:A:SER:H    | 1:34:A:CYS:H   | 6        | 0.12          |
| (1,255) | 1:31:A:SER:H    | 1:34:A:CYS:H   | 11       | 0.12          |
| (1,255) | 1:31:A:SER:H    | 1:34:A:CYS:H   | 16       | 0.12          |
| (1,255) | 1:31:A:SER:H    | 1:34:A:CYS:H   | 17       | 0.12          |
| (1,251) | 1:30:A:PRO:HG3  | 1:38:A:ALA:H   | 10       | 0.12          |
| (1,251) | 1:30:A:PRO:HG3  | 1:38:A:ALA:H   | 11       | 0.12          |
| (1,240) | 1:28:A:GLN:HB2  | 1:37:A:PRO:HA  | 16       | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,240) | 1:28:A:GLN:HB3 | 1:37:A:PRO:HA   | 16       | 0.12          |
| (1,210) | 1:26:A:ARG:HD2 | 1:40:A:LEU:HD11 | 5        | 0.12          |
| (1,210) | 1:26:A:ARG:HD2 | 1:40:A:LEU:HD12 | 5        | 0.12          |
| (1,210) | 1:26:A:ARG:HD2 | 1:40:A:LEU:HD13 | 5        | 0.12          |
| (1,210) | 1:26:A:ARG:HD2 | 1:40:A:LEU:HD21 | 5        | 0.12          |
| (1,210) | 1:26:A:ARG:HD2 | 1:40:A:LEU:HD22 | 5        | 0.12          |
| (1,210) | 1:26:A:ARG:HD2 | 1:40:A:LEU:HD23 | 5        | 0.12          |
| (1,210) | 1:26:A:ARG:HD3 | 1:40:A:LEU:HD11 | 5        | 0.12          |
| (1,210) | 1:26:A:ARG:HD3 | 1:40:A:LEU:HD12 | 5        | 0.12          |
| (1,210) | 1:26:A:ARG:HD3 | 1:40:A:LEU:HD13 | 5        | 0.12          |
| (1,210) | 1:26:A:ARG:HD3 | 1:40:A:LEU:HD21 | 5        | 0.12          |
| (1,210) | 1:26:A:ARG:HD3 | 1:40:A:LEU:HD22 | 5        | 0.12          |
| (1,210) | 1:26:A:ARG:HD3 | 1:40:A:LEU:HD23 | 5        | 0.12          |
| (1,200) | 1:26:A:ARG:H   | 1:40:A:LEU:HD11 | 8        | 0.12          |
| (1,200) | 1:26:A:ARG:H   | 1:40:A:LEU:HD12 | 8        | 0.12          |
| (1,200) | 1:26:A:ARG:H   | 1:40:A:LEU:HD13 | 8        | 0.12          |
| (1,200) | 1:26:A:ARG:H   | 1:40:A:LEU:HD21 | 8        | 0.12          |
| (1,200) | 1:26:A:ARG:H   | 1:40:A:LEU:HD22 | 8        | 0.12          |
| (1,200) | 1:26:A:ARG:H   | 1:40:A:LEU:HD23 | 8        | 0.12          |
| (1,200) | 1:26:A:ARG:H   | 1:40:A:LEU:HD11 | 14       | 0.12          |
| (1,200) | 1:26:A:ARG:H   | 1:40:A:LEU:HD12 | 14       | 0.12          |
| (1,200) | 1:26:A:ARG:H   | 1:40:A:LEU:HD13 | 14       | 0.12          |
| (1,200) | 1:26:A:ARG:H   | 1:40:A:LEU:HD21 | 14       | 0.12          |
| (1,200) | 1:26:A:ARG:H   | 1:40:A:LEU:HD22 | 14       | 0.12          |
| (1,200) | 1:26:A:ARG:H   | 1:40:A:LEU:HD23 | 14       | 0.12          |
| (1,152) | 1:23:A:ARG:HA  | 1:23:A:ARG:HD2  | 2        | 0.12          |
| (1,152) | 1:23:A:ARG:HA  | 1:23:A:ARG:HD3  | 2        | 0.12          |
| (1,152) | 1:23:A:ARG:HA  | 1:23:A:ARG:HD2  | 19       | 0.12          |
| (1,152) | 1:23:A:ARG:HA  | 1:23:A:ARG:HD3  | 19       | 0.12          |
| (1,121) | 1:20:A:LYS:HG2 | 1:21:A:VAL:H    | 1        | 0.12          |
| (1,121) | 1:20:A:LYS:HG3 | 1:21:A:VAL:H    | 1        | 0.12          |
| (1,121) | 1:20:A:LYS:HG2 | 1:21:A:VAL:H    | 3        | 0.12          |
| (1,121) | 1:20:A:LYS:HG3 | 1:21:A:VAL:H    | 3        | 0.12          |
| (1,97)  | 1:19:A:ALA:H   | 1:63:A:LEU:HG   | 3        | 0.12          |
| (1,97)  | 1:19:A:ALA:H   | 1:63:A:LEU:HG   | 4        | 0.12          |
| (1,97)  | 1:19:A:ALA:H   | 1:63:A:LEU:HG   | 12       | 0.12          |
| (1,97)  | 1:19:A:ALA:H   | 1:63:A:LEU:HG   | 13       | 0.12          |
| (1,97)  | 1:19:A:ALA:H   | 1:63:A:LEU:HG   | 15       | 0.12          |
| (1,81)  | 1:16:A:LYS:HB2 | 1:16:A:LYS:HD2  | 9        | 0.12          |
| (1,81)  | 1:16:A:LYS:HB2 | 1:16:A:LYS:HD3  | 9        | 0.12          |
| (1,81)  | 1:16:A:LYS:HB3 | 1:16:A:LYS:HD2  | 9        | 0.12          |
| (1,81)  | 1:16:A:LYS:HB3 | 1:16:A:LYS:HD3  | 9        | 0.12          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,69)  | 1:15:A:ARG:HA   | 1:15:A:ARG:HD2 | 7        | 0.12          |
| (1,69)  | 1:15:A:ARG:HA   | 1:15:A:ARG:HD3 | 7        | 0.12          |
| (1,69)  | 1:15:A:ARG:HA   | 1:15:A:ARG:HD2 | 16       | 0.12          |
| (1,69)  | 1:15:A:ARG:HA   | 1:15:A:ARG:HD3 | 16       | 0.12          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 8        | 0.12          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 8        | 0.12          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 8        | 0.12          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 8        | 0.12          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 8        | 0.12          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 8        | 0.12          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 8        | 0.12          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 8        | 0.12          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 8        | 0.12          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 8        | 0.12          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 8        | 0.12          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 8        | 0.12          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2 | 13       | 0.12          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3 | 13       | 0.12          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2 | 13       | 0.12          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3 | 13       | 0.12          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2 | 13       | 0.12          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3 | 13       | 0.12          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2 | 13       | 0.12          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3 | 13       | 0.12          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2 | 13       | 0.12          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3 | 13       | 0.12          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2 | 13       | 0.12          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3 | 13       | 0.12          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB1 | 6        | 0.12          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB2 | 6        | 0.12          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB3 | 6        | 0.12          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB1 | 6        | 0.12          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB2 | 6        | 0.12          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB3 | 6        | 0.12          |
| (1,16)  | 1:8:A:CYS:HA    | 1:9:A:CYS:H    | 13       | 0.12          |
| (1,568) | 1:67:A:LEU:HA   | 1:69:A:LYS:H   | 4        | 0.11          |
| (1,568) | 1:67:A:LEU:HA   | 1:69:A:LYS:H   | 7        | 0.11          |
| (1,568) | 1:67:A:LEU:HA   | 1:69:A:LYS:H   | 9        | 0.11          |
| (1,447) | 1:56:A:LYS:H    | 1:56:A:LYS:HG2 | 4        | 0.11          |
| (1,447) | 1:56:A:LYS:H    | 1:56:A:LYS:HG3 | 4        | 0.11          |
| (1,447) | 1:56:A:LYS:H    | 1:56:A:LYS:HG2 | 8        | 0.11          |
| (1,447) | 1:56:A:LYS:H    | 1:56:A:LYS:HG3 | 8        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,447) | 1:56:A:LYS:H    | 1:56:A:LYS:HG2  | 12       | 0.11          |
| (1,447) | 1:56:A:LYS:H    | 1:56:A:LYS:HG3  | 12       | 0.11          |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H    | 18       | 0.11          |
| (1,416) | 1:50:A:GLU:HG2  | 1:51:A:LEU:H    | 12       | 0.11          |
| (1,416) | 1:50:A:GLU:HG3  | 1:51:A:LEU:H    | 12       | 0.11          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB1  | 3        | 0.11          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB2  | 3        | 0.11          |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB3  | 3        | 0.11          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB1  | 13       | 0.11          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB2  | 13       | 0.11          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB3  | 13       | 0.11          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB1  | 19       | 0.11          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB2  | 19       | 0.11          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB3  | 19       | 0.11          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB1  | 20       | 0.11          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB2  | 20       | 0.11          |
| (1,340) | 1:41:A:PHE:HB2  | 1:53:A:ALA:HB3  | 20       | 0.11          |
| (1,323) | 1:40:A:LEU:HD21 | 1:52:A:CYS:H    | 17       | 0.11          |
| (1,323) | 1:40:A:LEU:HD22 | 1:52:A:CYS:H    | 17       | 0.11          |
| (1,323) | 1:40:A:LEU:HD23 | 1:52:A:CYS:H    | 17       | 0.11          |
| (1,321) | 1:40:A:LEU:HD11 | 1:52:A:CYS:H    | 5        | 0.11          |
| (1,321) | 1:40:A:LEU:HD12 | 1:52:A:CYS:H    | 5        | 0.11          |
| (1,321) | 1:40:A:LEU:HD13 | 1:52:A:CYS:H    | 5        | 0.11          |
| (1,300) | 1:39:A:ILE:HD11 | 1:64:A:MET:H    | 11       | 0.11          |
| (1,300) | 1:39:A:ILE:HD12 | 1:64:A:MET:H    | 11       | 0.11          |
| (1,300) | 1:39:A:ILE:HD13 | 1:64:A:MET:H    | 11       | 0.11          |
| (1,300) | 1:39:A:ILE:HD11 | 1:64:A:MET:H    | 16       | 0.11          |
| (1,300) | 1:39:A:ILE:HD12 | 1:64:A:MET:H    | 16       | 0.11          |
| (1,300) | 1:39:A:ILE:HD13 | 1:64:A:MET:H    | 16       | 0.11          |
| (1,297) | 1:39:A:ILE:HD11 | 1:40:A:LEU:H    | 7        | 0.11          |
| (1,297) | 1:39:A:ILE:HD12 | 1:40:A:LEU:H    | 7        | 0.11          |
| (1,297) | 1:39:A:ILE:HD13 | 1:40:A:LEU:H    | 7        | 0.11          |
| (1,280) | 1:37:A:PRO:HG2  | 1:38:A:ALA:H    | 14       | 0.11          |
| (1,280) | 1:37:A:PRO:HG3  | 1:38:A:ALA:H    | 14       | 0.11          |
| (1,255) | 1:31:A:SER:H    | 1:34:A:CYS:H    | 2        | 0.11          |
| (1,255) | 1:31:A:SER:H    | 1:34:A:CYS:H    | 13       | 0.11          |
| (1,251) | 1:30:A:PRO:HG3  | 1:38:A:ALA:H    | 16       | 0.11          |
| (1,230) | 1:27:A:LYS:HG2  | 1:28:A:GLN:H    | 3        | 0.11          |
| (1,230) | 1:27:A:LYS:HG3  | 1:28:A:GLN:H    | 3        | 0.11          |
| (1,204) | 1:26:A:ARG:HA   | 1:26:A:ARG:HD2  | 11       | 0.11          |
| (1,204) | 1:26:A:ARG:HA   | 1:26:A:ARG:HD3  | 11       | 0.11          |
| (1,200) | 1:26:A:ARG:H    | 1:40:A:LEU:HD11 | 20       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,200) | 1:26:A:ARG:H    | 1:40:A:LEU:HD12 | 20       | 0.11          |
| (1,200) | 1:26:A:ARG:H    | 1:40:A:LEU:HD13 | 20       | 0.11          |
| (1,200) | 1:26:A:ARG:H    | 1:40:A:LEU:HD21 | 20       | 0.11          |
| (1,200) | 1:26:A:ARG:H    | 1:40:A:LEU:HD22 | 20       | 0.11          |
| (1,200) | 1:26:A:ARG:H    | 1:40:A:LEU:HD23 | 20       | 0.11          |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD11 | 14       | 0.11          |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD12 | 14       | 0.11          |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD13 | 14       | 0.11          |
| (1,183) | 1:25:A:TYR:HD1  | 1:63:A:LEU:HB2  | 12       | 0.11          |
| (1,183) | 1:25:A:TYR:HD1  | 1:63:A:LEU:HB3  | 12       | 0.11          |
| (1,183) | 1:25:A:TYR:HD2  | 1:63:A:LEU:HB2  | 12       | 0.11          |
| (1,183) | 1:25:A:TYR:HD2  | 1:63:A:LEU:HB3  | 12       | 0.11          |
| (1,179) | 1:25:A:TYR:HB3  | 1:41:A:PHE:HE1  | 18       | 0.11          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD2  | 1        | 0.11          |
| (1,152) | 1:23:A:ARG:HA   | 1:23:A:ARG:HD3  | 1        | 0.11          |
| (1,121) | 1:20:A:LYS:HG2  | 1:21:A:VAL:H    | 8        | 0.11          |
| (1,121) | 1:20:A:LYS:HG3  | 1:21:A:VAL:H    | 8        | 0.11          |
| (1,121) | 1:20:A:LYS:HG2  | 1:21:A:VAL:H    | 12       | 0.11          |
| (1,121) | 1:20:A:LYS:HG3  | 1:21:A:VAL:H    | 12       | 0.11          |
| (1,97)  | 1:19:A:ALA:H    | 1:63:A:LEU:HG   | 6        | 0.11          |
| (1,97)  | 1:19:A:ALA:H    | 1:63:A:LEU:HG   | 16       | 0.11          |
| (1,69)  | 1:15:A:ARG:HA   | 1:15:A:ARG:HD2  | 19       | 0.11          |
| (1,69)  | 1:15:A:ARG:HA   | 1:15:A:ARG:HD3  | 19       | 0.11          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB2  | 7        | 0.11          |
| (1,38)  | 1:10:A:LEU:HD11 | 1:51:A:LEU:HB3  | 7        | 0.11          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB2  | 7        | 0.11          |
| (1,38)  | 1:10:A:LEU:HD12 | 1:51:A:LEU:HB3  | 7        | 0.11          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB2  | 7        | 0.11          |
| (1,38)  | 1:10:A:LEU:HD13 | 1:51:A:LEU:HB3  | 7        | 0.11          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB2  | 7        | 0.11          |
| (1,38)  | 1:10:A:LEU:HD21 | 1:51:A:LEU:HB3  | 7        | 0.11          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB2  | 7        | 0.11          |
| (1,38)  | 1:10:A:LEU:HD22 | 1:51:A:LEU:HB3  | 7        | 0.11          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB2  | 7        | 0.11          |
| (1,38)  | 1:10:A:LEU:HD23 | 1:51:A:LEU:HB3  | 7        | 0.11          |
| (1,37)  | 1:10:A:LEU:HD11 | 1:50:A:GLU:HB2  | 1        | 0.11          |
| (1,37)  | 1:10:A:LEU:HD11 | 1:50:A:GLU:HB3  | 1        | 0.11          |
| (1,37)  | 1:10:A:LEU:HD12 | 1:50:A:GLU:HB2  | 1        | 0.11          |
| (1,37)  | 1:10:A:LEU:HD12 | 1:50:A:GLU:HB3  | 1        | 0.11          |
| (1,37)  | 1:10:A:LEU:HD13 | 1:50:A:GLU:HB2  | 1        | 0.11          |
| (1,37)  | 1:10:A:LEU:HD13 | 1:50:A:GLU:HB3  | 1        | 0.11          |
| (1,37)  | 1:10:A:LEU:HD21 | 1:50:A:GLU:HB2  | 1        | 0.11          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,37)  | 1:10:A:LEU:HD21 | 1:50:A:GLU:HB3 | 1        | 0.11          |
| (1,37)  | 1:10:A:LEU:HD22 | 1:50:A:GLU:HB2 | 1        | 0.11          |
| (1,37)  | 1:10:A:LEU:HD22 | 1:50:A:GLU:HB3 | 1        | 0.11          |
| (1,37)  | 1:10:A:LEU:HD23 | 1:50:A:GLU:HB2 | 1        | 0.11          |
| (1,37)  | 1:10:A:LEU:HD23 | 1:50:A:GLU:HB3 | 1        | 0.11          |
| (1,37)  | 1:10:A:LEU:HD11 | 1:50:A:GLU:HB2 | 18       | 0.11          |
| (1,37)  | 1:10:A:LEU:HD11 | 1:50:A:GLU:HB3 | 18       | 0.11          |
| (1,37)  | 1:10:A:LEU:HD12 | 1:50:A:GLU:HB2 | 18       | 0.11          |
| (1,37)  | 1:10:A:LEU:HD12 | 1:50:A:GLU:HB3 | 18       | 0.11          |
| (1,37)  | 1:10:A:LEU:HD13 | 1:50:A:GLU:HB2 | 18       | 0.11          |
| (1,37)  | 1:10:A:LEU:HD13 | 1:50:A:GLU:HB3 | 18       | 0.11          |
| (1,37)  | 1:10:A:LEU:HD21 | 1:50:A:GLU:HB2 | 18       | 0.11          |
| (1,37)  | 1:10:A:LEU:HD21 | 1:50:A:GLU:HB3 | 18       | 0.11          |
| (1,37)  | 1:10:A:LEU:HD22 | 1:50:A:GLU:HB2 | 18       | 0.11          |
| (1,37)  | 1:10:A:LEU:HD22 | 1:50:A:GLU:HB3 | 18       | 0.11          |
| (1,37)  | 1:10:A:LEU:HD23 | 1:50:A:GLU:HB2 | 18       | 0.11          |
| (1,37)  | 1:10:A:LEU:HD23 | 1:50:A:GLU:HB3 | 18       | 0.11          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB1 | 19       | 0.11          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB2 | 19       | 0.11          |
| (1,18)  | 1:8:A:CYS:HB2   | 1:38:A:ALA:HB3 | 19       | 0.11          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB1 | 19       | 0.11          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB2 | 19       | 0.11          |
| (1,18)  | 1:8:A:CYS:HB3   | 1:38:A:ALA:HB3 | 19       | 0.11          |
| (1,583) | 1:69:A:LYS:HA   | 1:69:A:LYS:HE2 | 19       | 0.1           |
| (1,583) | 1:69:A:LYS:HA   | 1:69:A:LYS:HE3 | 19       | 0.1           |
| (1,568) | 1:67:A:LEU:HA   | 1:69:A:LYS:H   | 5        | 0.1           |
| (1,513) | 1:61:A:GLN:H    | 1:61:A:GLN:HG2 | 1        | 0.1           |
| (1,513) | 1:61:A:GLN:H    | 1:61:A:GLN:HG3 | 1        | 0.1           |
| (1,472) | 1:57:A:GLU:HG2  | 1:58:A:LEU:H   | 7        | 0.1           |
| (1,472) | 1:57:A:GLU:HG3  | 1:58:A:LEU:H   | 7        | 0.1           |
| (1,450) | 1:56:A:LYS:HA   | 1:56:A:LYS:HE2 | 16       | 0.1           |
| (1,450) | 1:56:A:LYS:HA   | 1:56:A:LYS:HE3 | 16       | 0.1           |
| (1,449) | 1:56:A:LYS:HA   | 1:56:A:LYS:HD2 | 13       | 0.1           |
| (1,449) | 1:56:A:LYS:HA   | 1:56:A:LYS:HD3 | 13       | 0.1           |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H   | 3        | 0.1           |
| (1,442) | 1:55:A:PRO:HB2  | 1:56:A:LYS:H   | 6        | 0.1           |
| (1,391) | 1:46:A:ARG:HA   | 1:47:A:SER:H   | 7        | 0.1           |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB1 | 6        | 0.1           |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB2 | 6        | 0.1           |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB3 | 6        | 0.1           |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB1 | 13       | 0.1           |
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB2 | 13       | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,346) | 1:41:A:PHE:HE1  | 1:53:A:ALA:HB3  | 13       | 0.1           |
| (1,300) | 1:39:A:ILE:HD11 | 1:64:A:MET:H    | 3        | 0.1           |
| (1,300) | 1:39:A:ILE:HD12 | 1:64:A:MET:H    | 3        | 0.1           |
| (1,300) | 1:39:A:ILE:HD13 | 1:64:A:MET:H    | 3        | 0.1           |
| (1,297) | 1:39:A:ILE:HD11 | 1:40:A:LEU:H    | 4        | 0.1           |
| (1,297) | 1:39:A:ILE:HD12 | 1:40:A:LEU:H    | 4        | 0.1           |
| (1,297) | 1:39:A:ILE:HD13 | 1:40:A:LEU:H    | 4        | 0.1           |
| (1,280) | 1:37:A:PRO:HG2  | 1:38:A:ALA:H    | 7        | 0.1           |
| (1,280) | 1:37:A:PRO:HG3  | 1:38:A:ALA:H    | 7        | 0.1           |
| (1,251) | 1:30:A:PRO:HG3  | 1:38:A:ALA:H    | 14       | 0.1           |
| (1,214) | 1:27:A:LYS:H    | 1:27:A:LYS:HD2  | 10       | 0.1           |
| (1,214) | 1:27:A:LYS:H    | 1:27:A:LYS:HD3  | 10       | 0.1           |
| (1,214) | 1:27:A:LYS:H    | 1:27:A:LYS:HD2  | 16       | 0.1           |
| (1,214) | 1:27:A:LYS:H    | 1:27:A:LYS:HD3  | 16       | 0.1           |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD11 | 8        | 0.1           |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD12 | 8        | 0.1           |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD13 | 8        | 0.1           |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD11 | 12       | 0.1           |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD12 | 12       | 0.1           |
| (1,196) | 1:26:A:ARG:H    | 1:39:A:ILE:HD13 | 12       | 0.1           |
| (1,121) | 1:20:A:LYS:HG2  | 1:21:A:VAL:H    | 16       | 0.1           |
| (1,121) | 1:20:A:LYS:HG3  | 1:21:A:VAL:H    | 16       | 0.1           |
| (1,97)  | 1:19:A:ALA:H    | 1:63:A:LEU:HG   | 14       | 0.1           |
| (1,44)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HD2  | 9        | 0.1           |
| (1,44)  | 1:11:A:LYS:HB2  | 1:11:A:LYS:HD3  | 9        | 0.1           |
| (1,44)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HD2  | 9        | 0.1           |
| (1,44)  | 1:11:A:LYS:HB3  | 1:11:A:LYS:HD3  | 9        | 0.1           |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD2  | 7        | 0.1           |
| (1,39)  | 1:11:A:LYS:H    | 1:11:A:LYS:HD3  | 7        | 0.1           |
| (1,13)  | 1:8:A:CYS:CB    | 1:34:A:CYS:CB   | 12       | 0.1           |

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

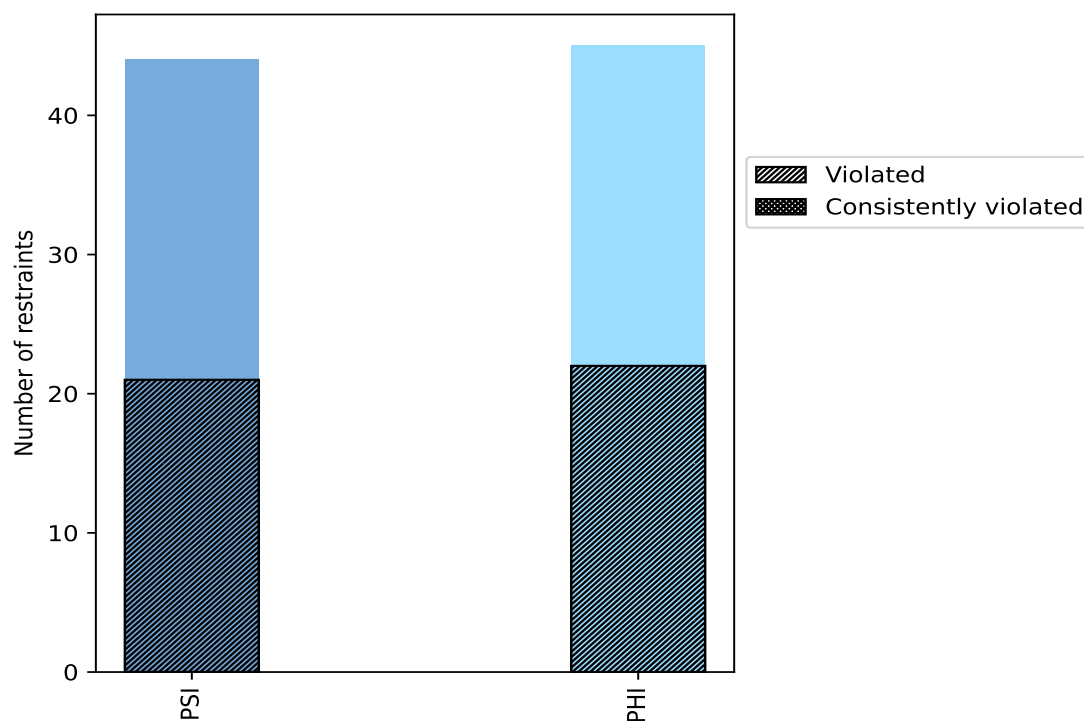
### 10.1 Summary of dihedral-angle violations [i](#)

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        | 44    | 49.4           | 21                    | 47.7           | 23.6           | 0                                  | 0.0            | 0.0            |
| PHI        | 45    | 50.6           | 22                    | 48.9           | 24.7           | 0                                  | 0.0            | 0.0            |
| Total      | 89    | 100.0          | 43                    | 48.3           | 48.3           | 0                                  | 0.0            | 0.0            |

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

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



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

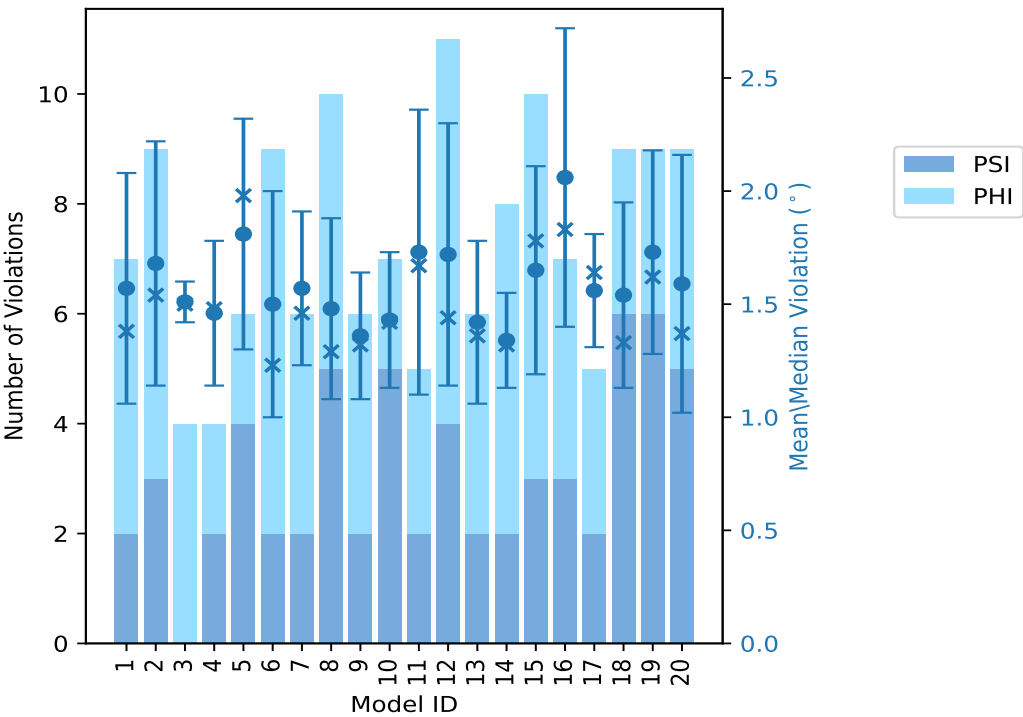
## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 2                    | 5   | 7     | 1.57     | 2.78    | 0.51   | 1.38       |
| 2        | 3                    | 6   | 9     | 1.68     | 2.42    | 0.54   | 1.54       |
| 3        | 0                    | 4   | 4     | 1.51     | 1.64    | 0.09   | 1.5        |
| 4        | 2                    | 2   | 4     | 1.46     | 1.85    | 0.32   | 1.48       |
| 5        | 4                    | 2   | 6     | 1.81     | 2.48    | 0.51   | 1.98       |
| 6        | 2                    | 7   | 9     | 1.5      | 2.57    | 0.5    | 1.23       |
| 7        | 2                    | 4   | 6     | 1.57     | 2.17    | 0.34   | 1.46       |
| 8        | 5                    | 5   | 10    | 1.48     | 2.47    | 0.4    | 1.29       |
| 9        | 2                    | 4   | 6     | 1.36     | 1.72    | 0.28   | 1.32       |
| 10       | 5                    | 2   | 7     | 1.43     | 1.94    | 0.3    | 1.42       |
| 11       | 2                    | 3   | 5     | 1.73     | 2.61    | 0.63   | 1.67       |
| 12       | 4                    | 7   | 11    | 1.72     | 3.15    | 0.58   | 1.44       |
| 13       | 2                    | 4   | 6     | 1.42     | 1.9     | 0.36   | 1.36       |
| 14       | 2                    | 6   | 8     | 1.34     | 1.66    | 0.21   | 1.32       |
| 15       | 3                    | 7   | 10    | 1.65     | 2.18    | 0.46   | 1.78       |
| 16       | 3                    | 4   | 7     | 2.06     | 3.09    | 0.66   | 1.83       |
| 17       | 2                    | 3   | 5     | 1.56     | 1.82    | 0.25   | 1.64       |
| 18       | 6                    | 3   | 9     | 1.54     | 2.29    | 0.41   | 1.33       |
| 19       | 6                    | 3   | 9     | 1.73     | 2.53    | 0.45   | 1.62       |
| 20       | 5                    | 4   | 9     | 1.59     | 2.65    | 0.57   | 1.37       |



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

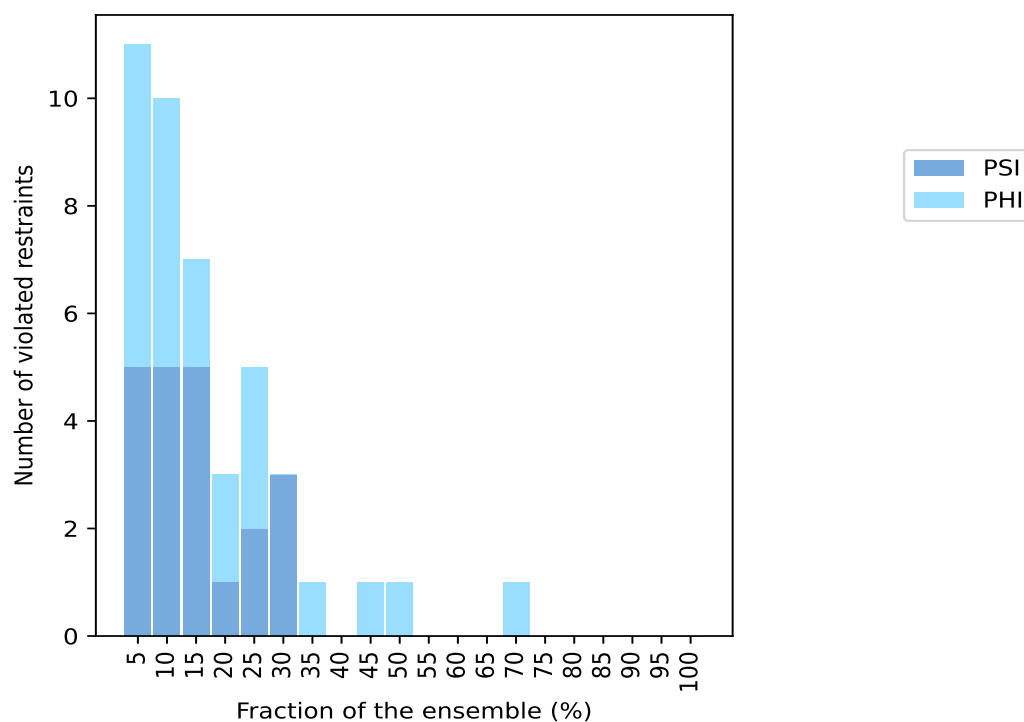
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0     | 12                       | 60.0  |
| 0                             | 0   | 0     | 13                       | 65.0  |
| 0                             | 1   | 1     | 14                       | 70.0  |
| 0                             | 0   | 0     | 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  |
| 0                             | 0   | 0     | 20                       | 100.0 |

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

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

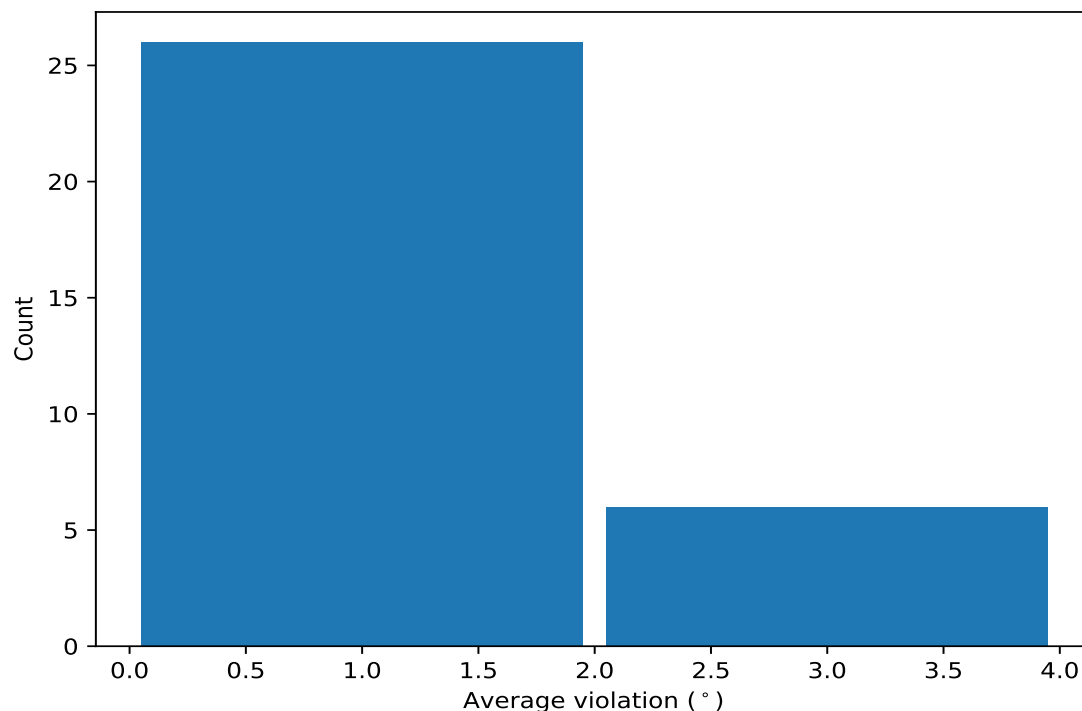


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



#### 10.4.2 Table: Most violated dihedral-angle restraints [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 |
|--------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 14                  | 1.5  | 0.26            | 1.51   |
| (1,16) | 1:16:A:LYS:C | 1:17:A:ILE:N  | 1:17:A:ILE:CA | 1:17:A:ILE:C | 10                  | 1.64 | 0.38            | 1.66   |
| (1,3)  | 1:9:A:CYS:C  | 1:10:A:LEU:N  | 1:10:A:LEU:CA | 1:10:A:LEU:C | 9                   | 1.65 | 0.46            | 1.54   |
| (1,27) | 1:26:A:ARG:C | 1:27:A:LYS:N  | 1:27:A:LYS:CA | 1:27:A:LYS:C | 7                   | 1.45 | 0.37            | 1.34   |
| (1,5)  | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C  | 1:12:A:TYR:N | 6                   | 2.22 | 0.44            | 2.1    |
| (1,84) | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C  | 1:68:A:ASP:N | 6                   | 1.48 | 0.3             | 1.38   |
| (1,60) | 1:52:A:CYS:N | 1:52:A:CYS:CA | 1:52:A:CYS:C  | 1:53:A:ALA:N | 6                   | 1.25 | 0.21            | 1.2    |
| (1,2)  | 1:7:A:ASP:N  | 1:7:A:ASP:CA  | 1:7:A:ASP:C   | 1:8:A:CYS:N  | 5                   | 1.79 | 0.44            | 1.53   |
| (1,58) | 1:50:A:GLU:C | 1:51:A:LEU:N  | 1:51:A:LEU:CA | 1:51:A:LEU:C | 5                   | 1.57 | 0.5             | 1.28   |
| (1,7)  | 1:12:A:TYR:N | 1:12:A:TYR:CA | 1:12:A:TYR:C  | 1:13:A:SER:N | 5                   | 1.48 | 0.36            | 1.24   |
| (1,78) | 1:63:A:LEU:C | 1:64:A:MET:N  | 1:64:A:MET:CA | 1:64:A:MET:C | 5                   | 1.4  | 0.44            | 1.21   |
| (1,52) | 1:43:A:PRO:C | 1:44:A:ARG:N  | 1:44:A:ARG:CA | 1:44:A:ARG:C | 5                   | 1.37 | 0.34            | 1.23   |
| (1,36) | 1:33:A:GLY:C | 1:34:A:CYS:N  | 1:34:A:CYS:CA | 1:34:A:CYS:C | 4                   | 1.59 | 0.36            | 1.52   |
| (1,24) | 1:22:A:VAL:N | 1:22:A:VAL:CA | 1:22:A:VAL:C  | 1:23:A:ARG:N | 4                   | 1.49 | 0.6             | 1.23   |
| (1,4)  | 1:10:A:LEU:C | 1:11:A:LYS:N  | 1:11:A:LYS:CA | 1:11:A:LYS:C | 4                   | 1.48 | 0.47            | 1.27   |
| (1,32) | 1:30:A:PRO:C | 1:31:A:SER:N  | 1:31:A:SER:CA | 1:31:A:SER:C | 3                   | 2.05 | 0.31            | 2.11   |
| (1,9)  | 1:13:A:SER:N | 1:13:A:SER:CA | 1:13:A:SER:C  | 1:14:A:GLN:N | 3                   | 1.79 | 0.58            | 1.46   |
| (1,86) | 1:68:A:ASP:N | 1:68:A:ASP:CA | 1:68:A:ASP:C  | 1:69:A:LYS:N | 3                   | 1.57 | 0.23            | 1.51   |
| (1,18) | 1:18:A:PRO:N | 1:18:A:PRO:CA | 1:18:A:PRO:C  | 1:19:A:ALA:N | 3                   | 1.51 | 0.19            | 1.49   |
| (1,57) | 1:50:A:GLU:N | 1:50:A:GLU:CA | 1:50:A:GLU:C  | 1:51:A:LEU:N | 3                   | 1.41 | 0.47            | 1.14   |

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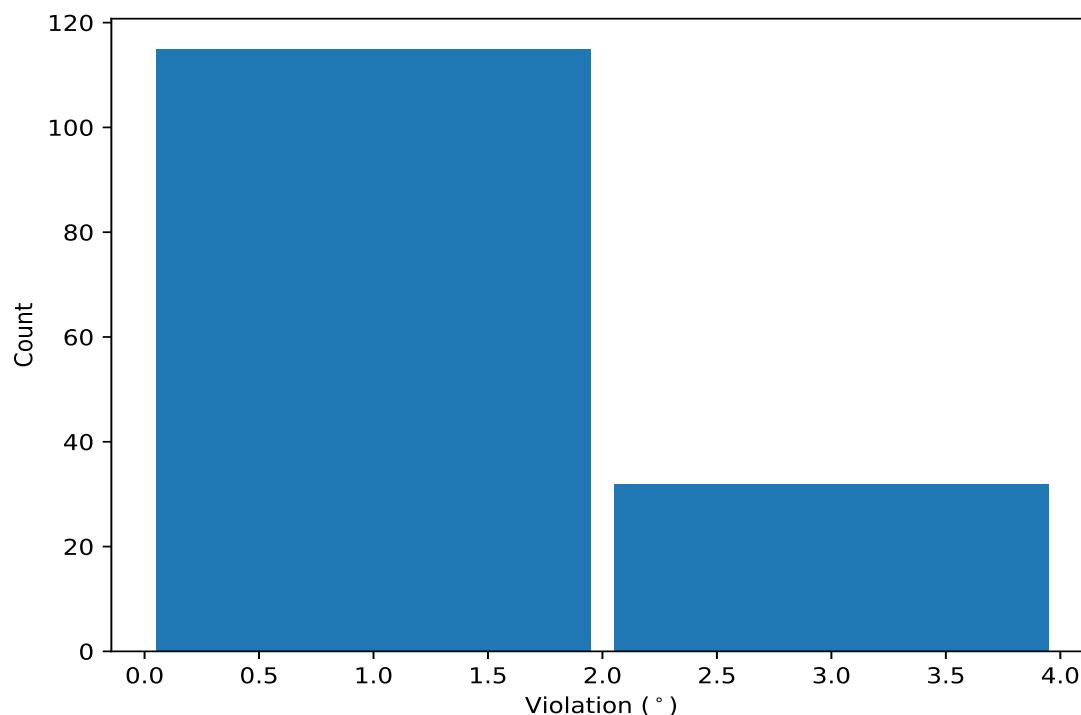
| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,53) | 1:44:A:ARG:C | 1:45:A:LYS:N  | 1:45:A:LYS:CA | 1:45:A:LYS:C | 3                   | 1.39 | 0.33            | 1.24   |
| (1,48) | 1:40:A:LEU:N | 1:40:A:LEU:CA | 1:40:A:LEU:C  | 1:41:A:PHE:N | 3                   | 1.27 | 0.08            | 1.32   |
| (1,34) | 1:31:A:SER:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C | 2                   | 2.22 | 0.35            | 2.22   |
| (1,28) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C  | 1:28:A:GLN:N | 2                   | 2.08 | 0.44            | 2.08   |
| (1,55) | 1:48:A:GLN:N | 1:48:A:GLN:CA | 1:48:A:GLN:C  | 1:49:A:ALA:N | 2                   | 2.08 | 0.01            | 2.08   |
| (1,29) | 1:27:A:LYS:C | 1:28:A:GLN:N  | 1:28:A:GLN:CA | 1:28:A:GLN:C | 2                   | 2.01 | 0.98            | 2.01   |
| (1,33) | 1:31:A:SER:N | 1:31:A:SER:CA | 1:31:A:SER:C  | 1:32:A:LEU:N | 2                   | 1.94 | 0.83            | 1.94   |
| (1,89) | 1:69:A:LYS:C | 1:70:A:THR:N  | 1:70:A:THR:CA | 1:70:A:THR:C | 2                   | 1.6  | 0.59            | 1.6    |
| (1,1)  | 1:6:A:GLN:C  | 1:7:A:ASP:N   | 1:7:A:ASP:CA  | 1:7:A:ASP:C  | 2                   | 1.56 | 0.3             | 1.56   |
| (1,88) | 1:69:A:LYS:N | 1:69:A:LYS:CA | 1:69:A:LYS:C  | 1:70:A:THR:N | 2                   | 1.44 | 0.26            | 1.44   |
| (1,25) | 1:25:A:TYR:N | 1:25:A:TYR:CA | 1:25:A:TYR:C  | 1:26:A:ARG:N | 2                   | 1.36 | 0.28            | 1.36   |
| (1,40) | 1:35:A:SER:C | 1:36:A:ILE:N  | 1:36:A:ILE:CA | 1:36:A:ILE:C | 2                   | 1.22 | 0.17            | 1.22   |

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

## 10.5 All violated dihedral-angle restraints ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,5)  | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C  | 1:12:A:TYR:N | 12       | 3.15          |
| (1,59) | 1:51:A:LEU:N | 1:51:A:LEU:CA | 1:51:A:LEU:C  | 1:52:A:CYS:N | 16       | 3.09          |
| (1,29) | 1:27:A:LYS:C | 1:28:A:GLN:N  | 1:28:A:GLN:CA | 1:28:A:GLN:C | 16       | 2.99          |
| (1,33) | 1:31:A:SER:N | 1:31:A:SER:CA | 1:31:A:SER:C  | 1:32:A:LEU:N | 1        | 2.78          |
| (1,3)  | 1:9:A:CYS:C  | 1:10:A:LEU:N  | 1:10:A:LEU:CA | 1:10:A:LEU:C | 20       | 2.65          |
| (1,9)  | 1:13:A:SER:N | 1:13:A:SER:CA | 1:13:A:SER:C  | 1:14:A:GLN:N | 11       | 2.61          |
| (1,34) | 1:31:A:SER:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C | 6        | 2.57          |
| (1,28) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C  | 1:28:A:GLN:N | 19       | 2.53          |
| (1,24) | 1:22:A:VAL:N | 1:22:A:VAL:CA | 1:22:A:VAL:C  | 1:23:A:ARG:N | 5        | 2.48          |
| (1,2)  | 1:7:A:ASP:N  | 1:7:A:ASP:CA  | 1:7:A:ASP:C   | 1:8:A:CYS:N  | 8        | 2.47          |
| (1,58) | 1:50:A:GLU:C | 1:51:A:LEU:N  | 1:51:A:LEU:CA | 1:51:A:LEU:C | 2        | 2.42          |
| (1,32) | 1:30:A:PRO:C | 1:31:A:SER:N  | 1:31:A:SER:CA | 1:31:A:SER:C | 12       | 2.39          |
| (1,77) | 1:63:A:LEU:N | 1:63:A:LEU:CA | 1:63:A:LEU:C  | 1:64:A:MET:N | 18       | 2.29          |
| (1,78) | 1:63:A:LEU:C | 1:64:A:MET:N  | 1:64:A:MET:CA | 1:64:A:MET:C | 2        | 2.26          |
| (1,4)  | 1:10:A:LEU:C | 1:11:A:LYS:N  | 1:11:A:LYS:CA | 1:11:A:LYS:C | 11       | 2.26          |
| (1,5)  | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C  | 1:12:A:TYR:N | 2        | 2.24          |
| (1,89) | 1:69:A:LYS:C | 1:70:A:THR:N  | 1:70:A:THR:CA | 1:70:A:THR:C | 15       | 2.18          |
| (1,36) | 1:33:A:GLY:C | 1:34:A:CYS:N  | 1:34:A:CYS:CA | 1:34:A:CYS:C | 7        | 2.17          |
| (1,27) | 1:26:A:ARG:C | 1:27:A:LYS:N  | 1:27:A:LYS:CA | 1:27:A:LYS:C | 15       | 2.16          |
| (1,16) | 1:16:A:LYS:C | 1:17:A:ILE:N  | 1:17:A:ILE:CA | 1:17:A:ILE:C | 20       | 2.15          |
| (1,5)  | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C  | 1:12:A:TYR:N | 19       | 2.15          |
| (1,2)  | 1:7:A:ASP:N  | 1:7:A:ASP:CA  | 1:7:A:ASP:C   | 1:8:A:CYS:N  | 19       | 2.15          |
| (1,7)  | 1:12:A:TYR:N | 1:12:A:TYR:CA | 1:12:A:TYR:C  | 1:13:A:SER:N | 5        | 2.14          |
| (1,32) | 1:30:A:PRO:C | 1:31:A:SER:N  | 1:31:A:SER:CA | 1:31:A:SER:C | 15       | 2.11          |
| (1,84) | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C  | 1:68:A:ASP:N | 6        | 2.1           |
| (1,16) | 1:16:A:LYS:C | 1:17:A:ILE:N  | 1:17:A:ILE:CA | 1:17:A:ILE:C | 2        | 2.1           |
| (1,55) | 1:48:A:GLN:N | 1:48:A:GLN:CA | 1:48:A:GLN:C  | 1:49:A:ALA:N | 5        | 2.09          |
| (1,57) | 1:50:A:GLU:N | 1:50:A:GLU:CA | 1:50:A:GLU:C  | 1:51:A:LEU:N | 12       | 2.07          |
| (1,3)  | 1:9:A:CYS:C  | 1:10:A:LEU:N  | 1:10:A:LEU:CA | 1:10:A:LEU:C | 18       | 2.07          |
| (1,55) | 1:48:A:GLN:N | 1:48:A:GLN:CA | 1:48:A:GLN:C  | 1:49:A:ALA:N | 15       | 2.06          |
| (1,5)  | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C  | 1:12:A:TYR:N | 20       | 2.06          |
| (1,52) | 1:43:A:PRO:C | 1:44:A:ARG:N  | 1:44:A:ARG:CA | 1:44:A:ARG:C | 16       | 2.03          |
| (1,16) | 1:16:A:LYS:C | 1:17:A:ILE:N  | 1:17:A:ILE:CA | 1:17:A:ILE:C | 10       | 1.94          |
| (1,16) | 1:16:A:LYS:C | 1:17:A:ILE:N  | 1:17:A:ILE:CA | 1:17:A:ILE:C | 8        | 1.93          |
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 18       | 1.92          |
| (1,5)  | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C  | 1:12:A:TYR:N | 13       | 1.9           |
| (1,86) | 1:68:A:ASP:N | 1:68:A:ASP:CA | 1:68:A:ASP:C  | 1:69:A:LYS:N | 5        | 1.88          |
| (1,34) | 1:31:A:SER:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C | 15       | 1.87          |
| (1,58) | 1:50:A:GLU:C | 1:51:A:LEU:N  | 1:51:A:LEU:CA | 1:51:A:LEU:C | 13       | 1.86          |
| (1,1)  | 1:6:A:GLN:C  | 1:7:A:ASP:N   | 1:7:A:ASP:CA  | 1:7:A:ASP:C  | 12       | 1.86          |
| (1,53) | 1:44:A:ARG:C | 1:45:A:LYS:N  | 1:45:A:LYS:CA | 1:45:A:LYS:C | 4        | 1.85          |
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 19       | 1.84          |
| (1,37) | 1:34:A:CYS:N | 1:34:A:CYS:CA | 1:34:A:CYS:C  | 1:35:A:SER:N | 20       | 1.84          |
| (1,5)  | 1:11:A:LYS:N | 1:11:A:LYS:CA | 1:11:A:LYS:C  | 1:12:A:TYR:N | 16       | 1.83          |
| (1,27) | 1:26:A:ARG:C | 1:27:A:LYS:N  | 1:27:A:LYS:CA | 1:27:A:LYS:C | 17       | 1.82          |
| (1,3)  | 1:9:A:CYS:C  | 1:10:A:LEU:N  | 1:10:A:LEU:CA | 1:10:A:LEU:C | 7        | 1.8           |
| (1,18) | 1:18:A:PRO:N | 1:18:A:PRO:CA | 1:18:A:PRO:C  | 1:19:A:ALA:N | 17       | 1.75          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 16       | 1.73          |
| (1,3)  | 1:9:A:CYS:C  | 1:10:A:LEU:N  | 1:10:A:LEU:CA | 1:10:A:LEU:C | 9        | 1.72          |
| (1,88) | 1:69:A:LYS:N | 1:69:A:LYS:CA | 1:69:A:LYS:C  | 1:70:A:THR:N | 15       | 1.7           |
| (1,85) | 1:67:A:LEU:C | 1:68:A:ASP:N  | 1:68:A:ASP:CA | 1:68:A:ASP:C | 6        | 1.68          |
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 9        | 1.68          |
| (1,16) | 1:16:A:LYS:C | 1:17:A:ILE:N  | 1:17:A:ILE:CA | 1:17:A:ILE:C | 11       | 1.67          |
| (1,16) | 1:16:A:LYS:C | 1:17:A:ILE:N  | 1:17:A:ILE:CA | 1:17:A:ILE:C | 14       | 1.66          |
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 8        | 1.65          |
| (1,32) | 1:30:A:PRO:C | 1:31:A:SER:N  | 1:31:A:SER:CA | 1:31:A:SER:C | 3        | 1.64          |
| (1,28) | 1:27:A:LYS:N | 1:27:A:LYS:CA | 1:27:A:LYS:C  | 1:28:A:GLN:N | 17       | 1.64          |
| (1,25) | 1:25:A:TYR:N | 1:25:A:TYR:CA | 1:25:A:TYR:C  | 1:26:A:ARG:N | 4        | 1.64          |
| (1,60) | 1:52:A:CYS:N | 1:52:A:CYS:CA | 1:52:A:CYS:C  | 1:53:A:ALA:N | 19       | 1.62          |
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 10       | 1.62          |
| (1,7)  | 1:12:A:TYR:N | 1:12:A:TYR:CA | 1:12:A:TYR:C  | 1:13:A:SER:N | 10       | 1.61          |
| (1,16) | 1:16:A:LYS:C | 1:17:A:ILE:N  | 1:17:A:ILE:CA | 1:17:A:ILE:C | 19       | 1.55          |
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 2        | 1.54          |
| (1,36) | 1:33:A:GLY:C | 1:34:A:CYS:N  | 1:34:A:CYS:CA | 1:34:A:CYS:C | 12       | 1.54          |
| (1,3)  | 1:9:A:CYS:C  | 1:10:A:LEU:N  | 1:10:A:LEU:CA | 1:10:A:LEU:C | 1        | 1.54          |
| (1,3)  | 1:9:A:CYS:C  | 1:10:A:LEU:N  | 1:10:A:LEU:CA | 1:10:A:LEU:C | 14       | 1.54          |
| (1,2)  | 1:7:A:ASP:N  | 1:7:A:ASP:CA  | 1:7:A:ASP:C   | 1:8:A:CYS:N  | 14       | 1.53          |
| (1,86) | 1:68:A:ASP:N | 1:68:A:ASP:CA | 1:68:A:ASP:C  | 1:69:A:LYS:N | 1        | 1.51          |
| (1,38) | 1:34:A:CYS:C | 1:35:A:SER:N  | 1:35:A:SER:CA | 1:35:A:SER:C | 3        | 1.51          |
| (1,84) | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C  | 1:68:A:ASP:N | 16       | 1.5           |
| (1,36) | 1:33:A:GLY:C | 1:34:A:CYS:N  | 1:34:A:CYS:CA | 1:34:A:CYS:C | 3        | 1.5           |
| (1,18) | 1:18:A:PRO:N | 1:18:A:PRO:CA | 1:18:A:PRO:C  | 1:19:A:ALA:N | 13       | 1.49          |
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 17       | 1.48          |
| (1,27) | 1:26:A:ARG:C | 1:27:A:LYS:N  | 1:27:A:LYS:CA | 1:27:A:LYS:C | 7        | 1.47          |
| (1,21) | 1:20:A:LYS:C | 1:21:A:VAL:N  | 1:21:A:VAL:CA | 1:21:A:VAL:C | 9        | 1.47          |
| (1,9)  | 1:13:A:SER:N | 1:13:A:SER:CA | 1:13:A:SER:C  | 1:14:A:GLN:N | 7        | 1.46          |
| (1,24) | 1:22:A:VAL:N | 1:22:A:VAL:CA | 1:22:A:VAL:C  | 1:23:A:ARG:N | 18       | 1.45          |
| (1,84) | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C  | 1:68:A:ASP:N | 12       | 1.44          |
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 6        | 1.44          |
| (1,60) | 1:52:A:CYS:N | 1:52:A:CYS:CA | 1:52:A:CYS:C  | 1:53:A:ALA:N | 7        | 1.42          |
| (1,2)  | 1:7:A:ASP:N  | 1:7:A:ASP:CA  | 1:7:A:ASP:C   | 1:8:A:CYS:N  | 10       | 1.42          |
| (1,40) | 1:35:A:SER:C | 1:36:A:ILE:N  | 1:36:A:ILE:CA | 1:36:A:ILE:C | 12       | 1.39          |
| (1,2)  | 1:7:A:ASP:N  | 1:7:A:ASP:CA  | 1:7:A:ASP:C   | 1:8:A:CYS:N  | 12       | 1.39          |
| (1,19) | 1:19:A:ALA:C | 1:20:A:LYS:N  | 1:20:A:LYS:CA | 1:20:A:LYS:C | 1        | 1.38          |
| (1,4)  | 1:10:A:LEU:C | 1:11:A:LYS:N  | 1:11:A:LYS:CA | 1:11:A:LYS:C | 3        | 1.38          |
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 20       | 1.37          |
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 14       | 1.35          |
| (1,27) | 1:26:A:ARG:C | 1:27:A:LYS:N  | 1:27:A:LYS:CA | 1:27:A:LYS:C | 12       | 1.34          |
| (1,84) | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C  | 1:68:A:ASP:N | 19       | 1.33          |
| (1,52) | 1:43:A:PRO:C | 1:44:A:ARG:N  | 1:44:A:ARG:CA | 1:44:A:ARG:C | 8        | 1.33          |
| (1,48) | 1:40:A:LEU:N | 1:40:A:LEU:CA | 1:40:A:LEU:C  | 1:41:A:PHE:N | 18       | 1.33          |
| (1,86) | 1:68:A:ASP:N | 1:68:A:ASP:CA | 1:68:A:ASP:C  | 1:69:A:LYS:N | 8        | 1.32          |
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 1        | 1.32          |
| (1,48) | 1:40:A:LEU:N | 1:40:A:LEU:CA | 1:40:A:LEU:C  | 1:41:A:PHE:N | 4        | 1.32          |
| (1,9)  | 1:13:A:SER:N | 1:13:A:SER:CA | 1:13:A:SER:C  | 1:14:A:GLN:N | 2        | 1.31          |
| (1,78) | 1:63:A:LEU:C | 1:64:A:MET:N  | 1:64:A:MET:CA | 1:64:A:MET:C | 1        | 1.3           |
| (1,18) | 1:18:A:PRO:N | 1:18:A:PRO:CA | 1:18:A:PRO:C  | 1:19:A:ALA:N | 19       | 1.29          |
| (1,58) | 1:50:A:GLU:C | 1:51:A:LEU:N  | 1:51:A:LEU:CA | 1:51:A:LEU:C | 14       | 1.28          |

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Continued from previous page...

| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,84) | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C  | 1:68:A:ASP:N | 10       | 1.27          |
| (1,3)  | 1:9:A:CYS:C  | 1:10:A:LEU:N  | 1:10:A:LEU:CA | 1:10:A:LEU:C | 16       | 1.26          |
| (1,1)  | 1:6:A:GLN:C  | 1:7:A:ASP:N   | 1:7:A:ASP:CA  | 1:7:A:ASP:C  | 8        | 1.26          |
| (1,60) | 1:52:A:CYS:N | 1:52:A:CYS:CA | 1:52:A:CYS:C  | 1:53:A:ALA:N | 14       | 1.24          |
| (1,53) | 1:44:A:ARG:C | 1:45:A:LYS:N  | 1:45:A:LYS:CA | 1:45:A:LYS:C | 13       | 1.24          |
| (1,7)  | 1:12:A:TYR:N | 1:12:A:TYR:CA | 1:12:A:TYR:C  | 1:13:A:SER:N | 8        | 1.24          |
| (1,83) | 1:66:A:HIS:C | 1:67:A:LEU:N  | 1:67:A:LEU:CA | 1:67:A:LEU:C | 2        | 1.23          |
| (1,58) | 1:50:A:GLU:C | 1:51:A:LEU:N  | 1:51:A:LEU:CA | 1:51:A:LEU:C | 5        | 1.23          |
| (1,52) | 1:43:A:PRO:C | 1:44:A:ARG:N  | 1:44:A:ARG:CA | 1:44:A:ARG:C | 6        | 1.23          |
| (1,16) | 1:16:A:LYS:C | 1:17:A:ILE:N  | 1:17:A:ILE:CA | 1:17:A:ILE:C | 18       | 1.23          |
| (1,7)  | 1:12:A:TYR:N | 1:12:A:TYR:CA | 1:12:A:TYR:C  | 1:13:A:SER:N | 18       | 1.23          |
| (1,3)  | 1:9:A:CYS:C  | 1:10:A:LEU:N  | 1:10:A:LEU:CA | 1:10:A:LEU:C | 12       | 1.23          |
| (1,84) | 1:67:A:LEU:N | 1:67:A:LEU:CA | 1:67:A:LEU:C  | 1:68:A:ASP:N | 8        | 1.21          |
| (1,78) | 1:63:A:LEU:C | 1:64:A:MET:N  | 1:64:A:MET:CA | 1:64:A:MET:C | 15       | 1.21          |
| (1,27) | 1:26:A:ARG:C | 1:27:A:LYS:N  | 1:27:A:LYS:CA | 1:27:A:LYS:C | 8        | 1.2           |
| (1,88) | 1:69:A:LYS:N | 1:69:A:LYS:CA | 1:69:A:LYS:C  | 1:70:A:THR:N | 8        | 1.19          |
| (1,7)  | 1:12:A:TYR:N | 1:12:A:TYR:CA | 1:12:A:TYR:C  | 1:13:A:SER:N | 20       | 1.18          |
| (1,60) | 1:52:A:CYS:N | 1:52:A:CYS:CA | 1:52:A:CYS:C  | 1:53:A:ALA:N | 18       | 1.16          |
| (1,48) | 1:40:A:LEU:N | 1:40:A:LEU:CA | 1:40:A:LEU:C  | 1:41:A:PHE:N | 9        | 1.16          |
| (1,36) | 1:33:A:GLY:C | 1:34:A:CYS:N  | 1:34:A:CYS:CA | 1:34:A:CYS:C | 6        | 1.16          |
| (1,4)  | 1:10:A:LEU:C | 1:11:A:LYS:N  | 1:11:A:LYS:CA | 1:11:A:LYS:C | 1        | 1.16          |
| (1,57) | 1:50:A:GLU:N | 1:50:A:GLU:CA | 1:50:A:GLU:C  | 1:51:A:LEU:N | 18       | 1.14          |
| (1,27) | 1:26:A:ARG:C | 1:27:A:LYS:N  | 1:27:A:LYS:CA | 1:27:A:LYS:C | 6        | 1.14          |
| (1,52) | 1:43:A:PRO:C | 1:44:A:ARG:N  | 1:44:A:ARG:CA | 1:44:A:ARG:C | 14       | 1.13          |
| (1,52) | 1:43:A:PRO:C | 1:44:A:ARG:N  | 1:44:A:ARG:CA | 1:44:A:ARG:C | 17       | 1.13          |
| (1,78) | 1:63:A:LEU:C | 1:64:A:MET:N  | 1:64:A:MET:CA | 1:64:A:MET:C | 12       | 1.12          |
| (1,15) | 1:16:A:LYS:N | 1:16:A:LYS:CA | 1:16:A:LYS:C  | 1:17:A:ILE:N | 10       | 1.12          |
| (1,78) | 1:63:A:LEU:C | 1:64:A:MET:N  | 1:64:A:MET:CA | 1:64:A:MET:C | 19       | 1.11          |
| (1,33) | 1:31:A:SER:N | 1:31:A:SER:CA | 1:31:A:SER:C  | 1:32:A:LEU:N | 15       | 1.11          |
| (1,4)  | 1:10:A:LEU:C | 1:11:A:LYS:N  | 1:11:A:LYS:CA | 1:11:A:LYS:C | 9        | 1.1           |
| (1,16) | 1:16:A:LYS:C | 1:17:A:ILE:N  | 1:17:A:ILE:CA | 1:17:A:ILE:C | 15       | 1.09          |
| (1,58) | 1:50:A:GLU:C | 1:51:A:LEU:N  | 1:51:A:LEU:CA | 1:51:A:LEU:C | 7        | 1.08          |
| (1,16) | 1:16:A:LYS:C | 1:17:A:ILE:N  | 1:17:A:ILE:CA | 1:17:A:ILE:C | 6        | 1.08          |
| (1,53) | 1:44:A:ARG:C | 1:45:A:LYS:N  | 1:45:A:LYS:CA | 1:45:A:LYS:C | 11       | 1.07          |
| (1,25) | 1:25:A:TYR:N | 1:25:A:TYR:CA | 1:25:A:TYR:C  | 1:26:A:ARG:N | 6        | 1.07          |
| (1,81) | 1:65:A:GLN:C | 1:66:A:HIS:N  | 1:66:A:HIS:CA | 1:66:A:HIS:C | 2        | 1.05          |
| (1,40) | 1:35:A:SER:C | 1:36:A:ILE:N  | 1:36:A:ILE:CA | 1:36:A:ILE:C | 15       | 1.05          |
| (1,27) | 1:26:A:ARG:C | 1:27:A:LYS:N  | 1:27:A:LYS:CA | 1:27:A:LYS:C | 20       | 1.04          |
| (1,11) | 1:14:A:GLN:N | 1:14:A:GLN:CA | 1:14:A:GLN:C  | 1:15:A:ARG:N | 20       | 1.04          |
| (1,3)  | 1:9:A:CYS:C  | 1:10:A:LEU:N  | 1:10:A:LEU:CA | 1:10:A:LEU:C | 5        | 1.04          |
| (1,60) | 1:52:A:CYS:N | 1:52:A:CYS:CA | 1:52:A:CYS:C  | 1:53:A:ALA:N | 9        | 1.03          |
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 13       | 1.03          |
| (1,29) | 1:27:A:LYS:C | 1:28:A:GLN:N  | 1:28:A:GLN:CA | 1:28:A:GLN:C | 13       | 1.03          |
| (1,60) | 1:52:A:CYS:N | 1:52:A:CYS:CA | 1:52:A:CYS:C  | 1:53:A:ALA:N | 10       | 1.02          |
| (1,24) | 1:22:A:VAL:N | 1:22:A:VAL:CA | 1:22:A:VAL:C  | 1:23:A:ARG:N | 11       | 1.02          |
| (1,89) | 1:69:A:LYS:C | 1:70:A:THR:N  | 1:70:A:THR:CA | 1:70:A:THR:C | 14       | 1.01          |
| (1,57) | 1:50:A:GLU:N | 1:50:A:GLU:CA | 1:50:A:GLU:C  | 1:51:A:LEU:N | 20       | 1.01          |
| (1,49) | 1:40:A:LEU:C | 1:41:A:PHE:N  | 1:41:A:PHE:CA | 1:41:A:PHE:C | 4        | 1.01          |
| (1,24) | 1:22:A:VAL:N | 1:22:A:VAL:CA | 1:22:A:VAL:C  | 1:23:A:ARG:N | 2        | 1.0           |