



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 24, 2026 – 11:33 AM UTC

PDB ID : 6EWV / pdb\_00006ewv  
BMRB ID : 34196  
Title : Solution Structure of Docking Domain Complex of RXP NRPS: Kj12C NDD  
- Kj12B CDD  
Authors : Hacker, C.; Cai, X.; Kegler, C.; Zhao, L.; Weickhmann, A.K.; Bode, H.B.;  
Woehnert, J.  
Deposited on : 2017-11-06

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

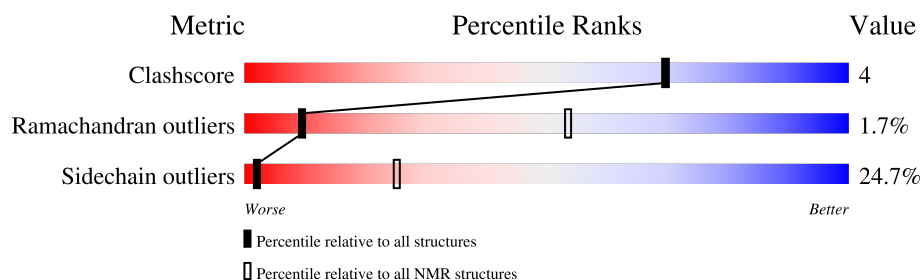
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 83%.

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



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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 99     |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues |                                 |                   |              |
|--------------------------------------|---------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)           | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:2-A:58, A:1563-A:1568<br>(63) | 0.25              | 1            |

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 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1540 atoms, of which 759 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NRPS Kj12C-NDD, NRPS Kj12B-CDD.

| Mol | Chain | Residues | Atoms |     |     |     |     | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|-------|
| 1   | A     | 99       | Total | C   | H   | N   | O   | 0     |
|     |       |          | 1540  | 480 | 759 | 138 | 163 |       |

There are 13 discrepancies between the modelled and reference sequences:

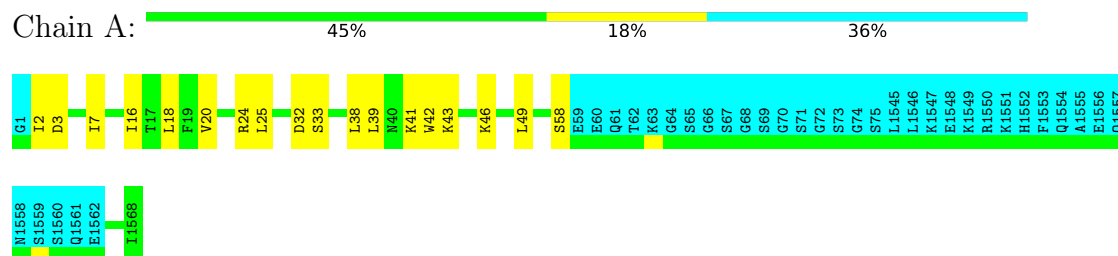
| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| A     | 1       | GLY      | -      | expression tag | UNP A0A173DW42 |
| A     | 64      | GLY      | -      | linker         | UNP A0A173DW42 |
| A     | 65      | SER      | -      | linker         | UNP A0A173DW42 |
| A     | 66      | GLY      | -      | linker         | UNP A0A173DW42 |
| A     | 67      | SER      | -      | linker         | UNP A0A173DW42 |
| A     | 68      | GLY      | -      | linker         | UNP A0A173DW42 |
| A     | 69      | SER      | -      | linker         | UNP A0A173DW42 |
| A     | 70      | GLY      | -      | linker         | UNP A0A173DW42 |
| A     | 71      | SER      | -      | linker         | UNP A0A173DW42 |
| A     | 72      | GLY      | -      | linker         | UNP A0A173DW42 |
| A     | 73      | SER      | -      | linker         | UNP A0A173DW42 |
| A     | 74      | GLY      | -      | linker         | UNP A0A173DW42 |
| A     | 75      | SER      | -      | linker         | UNP A0A173DW42 |

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

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

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

- Molecule 1: NRPS K<sub>j</sub>12C-NDD, NRPS K<sub>j</sub>12B-CDD

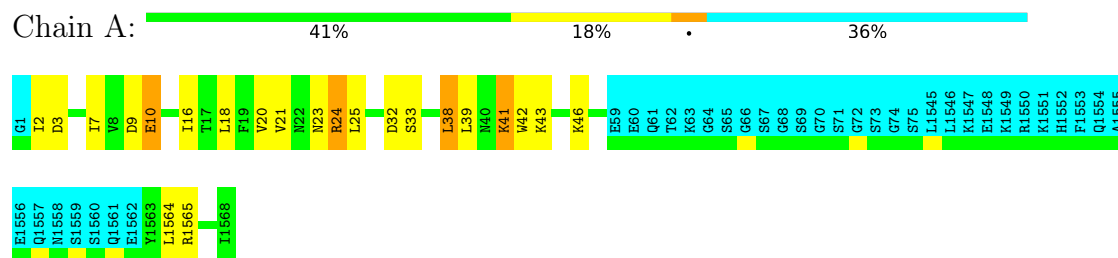


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

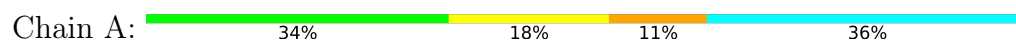
#### 4.2.1 Score per residue for model 1 (medoid)

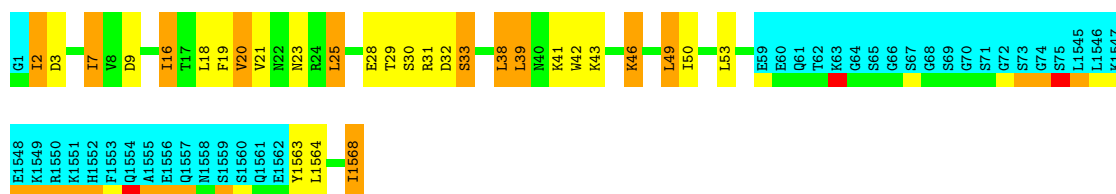
- Molecule 1: NRPS K<sub>j</sub>12C-NDD, NRPS K<sub>j</sub>12B-CDD



#### 4.2.2 Score per residue for model 2

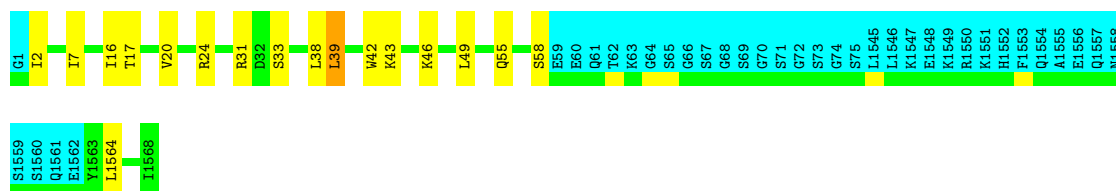
- Molecule 1: NRPS K<sub>j</sub>12C-NDD, NRPS K<sub>j</sub>12B-CDD





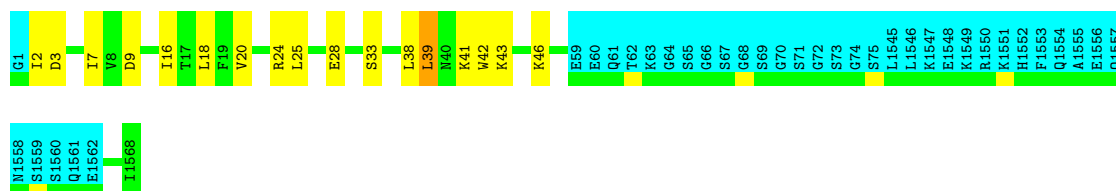
#### 4.2.3 Score per residue for model 3

- Molecule 1: NRPS K<sub>j</sub>12C-NDD, NRPS K<sub>j</sub>12B-CDD



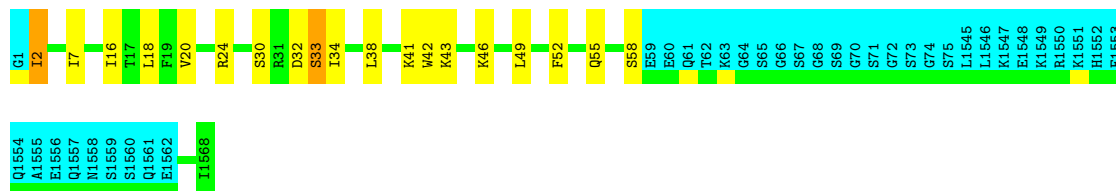
#### 4.2.4 Score per residue for model 4

- Molecule 1: NRPS K<sub>j</sub>12C-NDD, NRPS K<sub>j</sub>12B-CDD



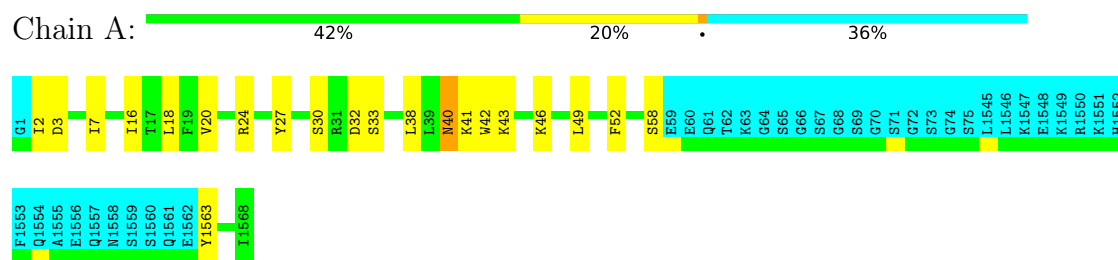
#### 4.2.5 Score per residue for model 5

- Molecule 1: NRPS K<sub>j</sub>12C-NDD, NRPS K<sub>j</sub>12B-CDD



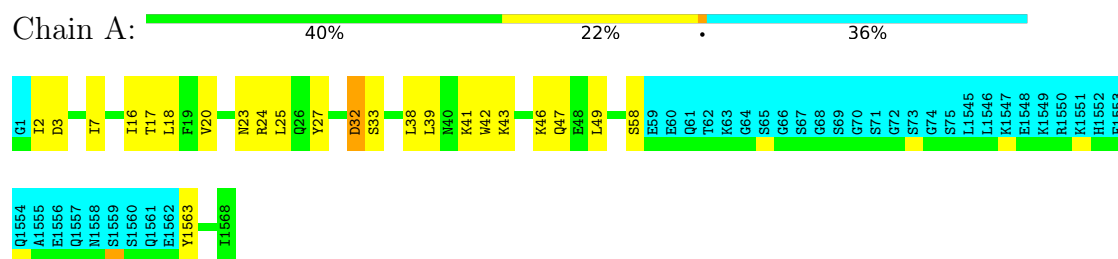
### 4.2.6 Score per residue for model 6

- Molecule 1: NRPS K<sub>j</sub>12C-NDD, NRPS K<sub>j</sub>12B-CDD



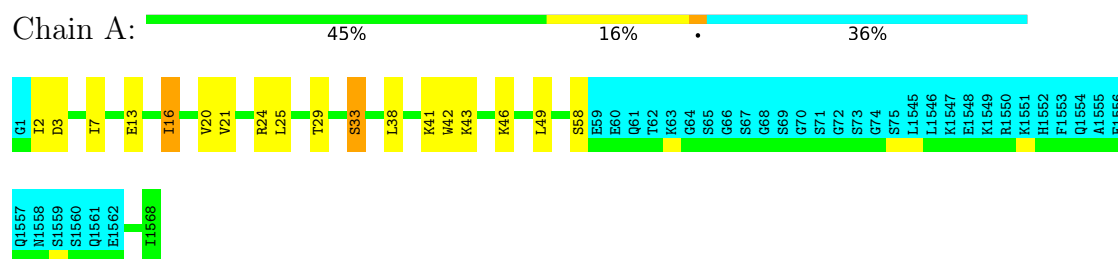
### 4.2.7 Score per residue for model 7

- Molecule 1: NRPS K<sub>j</sub>12C-NDD, NRPS K<sub>j</sub>12B-CDD



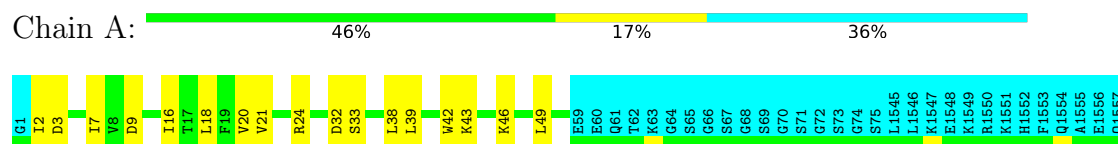
### 4.2.8 Score per residue for model 8

- Molecule 1: NRPS K<sub>j</sub>12C-NDD, NRPS K<sub>j</sub>12B-CDD



### 4.2.9 Score per residue for model 9

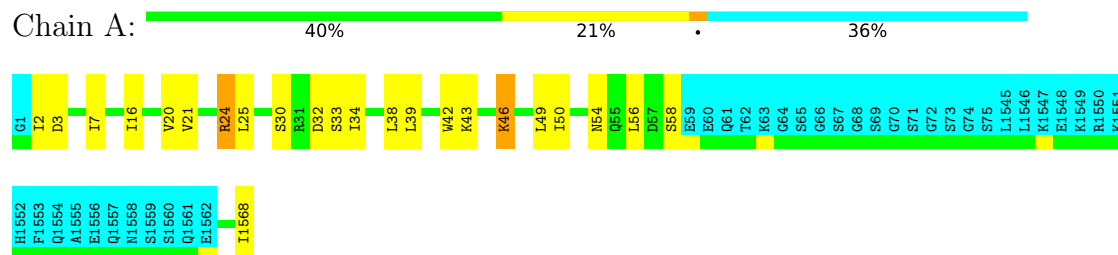
- Molecule 1: NRPS K<sub>j</sub>12C-NDD, NRPS K<sub>j</sub>12B-CDD





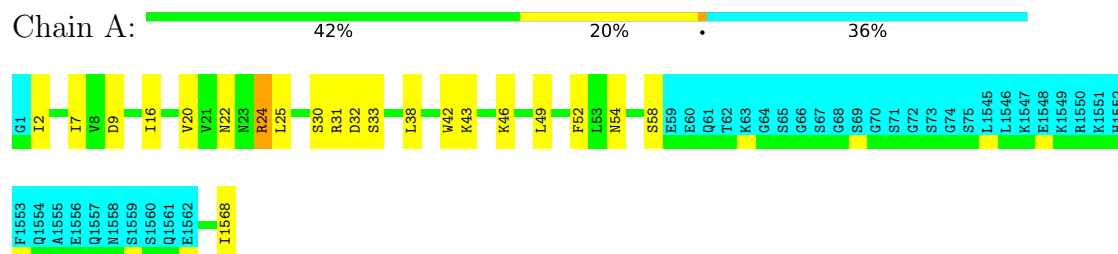
#### 4.2.10 Score per residue for model 10

- Molecule 1: NRPS Kj12C-NDD, NRPS Kj12B-CDD



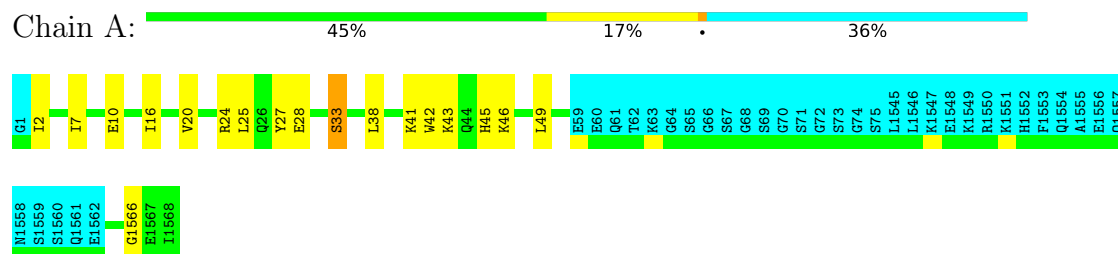
#### 4.2.11 Score per residue for model 11

- Molecule 1: NRPS Kj12C-NDD, NRPS Kj12B-CDD



#### 4.2.12 Score per residue for model 12

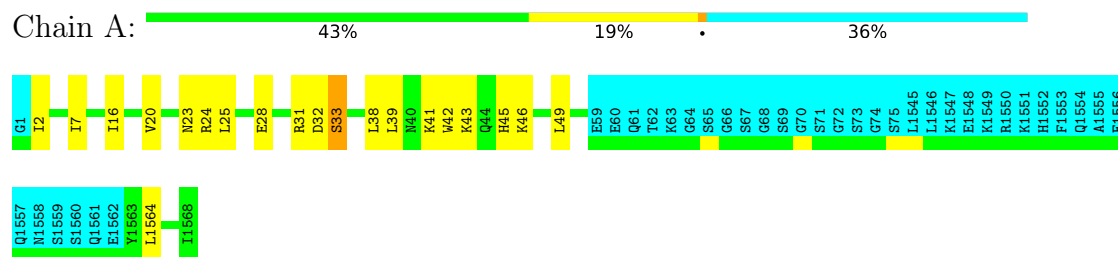
- Molecule 1: NRPS Kj12C-NDD, NRPS Kj12B-CDD



#### 4.2.13 Score per residue for model 13

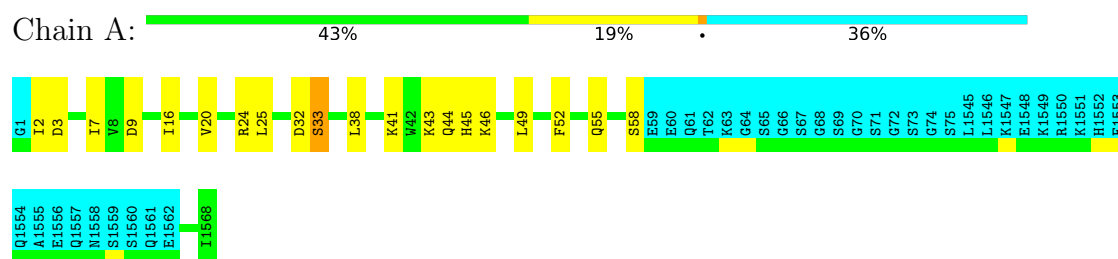
- Molecule 1: NRPS Kj12C-NDD, NRPS Kj12B-CDD





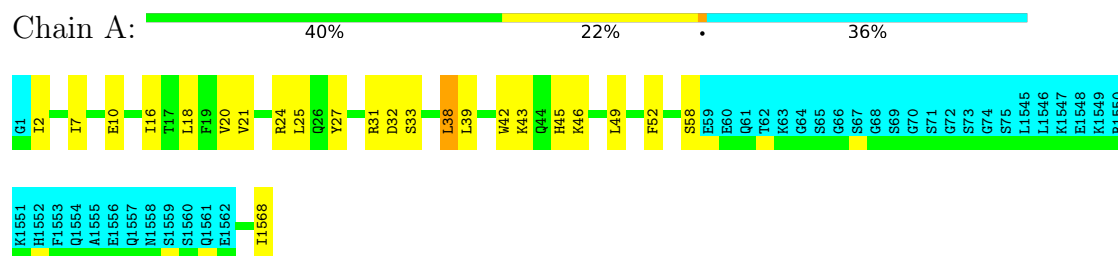
#### 4.2.14 Score per residue for model 14

- Molecule 1: NRPS Kj12C-NDD, NRPS Kj12B-CDD



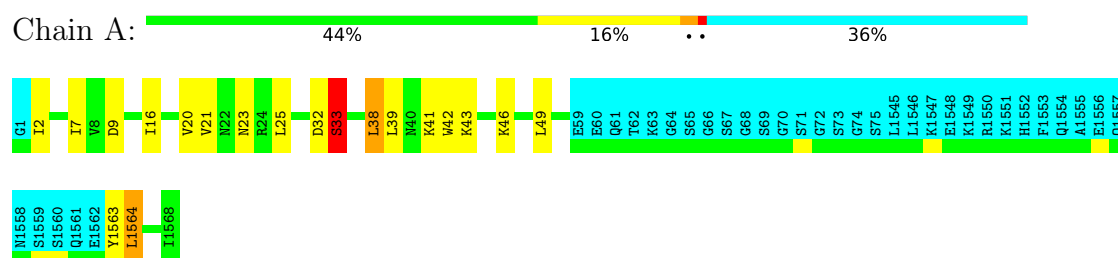
#### 4.2.15 Score per residue for model 15

- Molecule 1: NRPS Kj12C-NDD, NRPS Kj12B-CDD



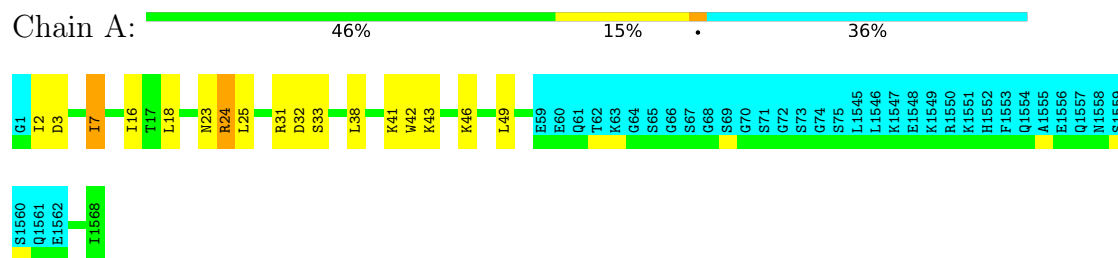
#### 4.2.16 Score per residue for model 16

- Molecule 1: NRPS Kj12C-NDD, NRPS Kj12B-CDD



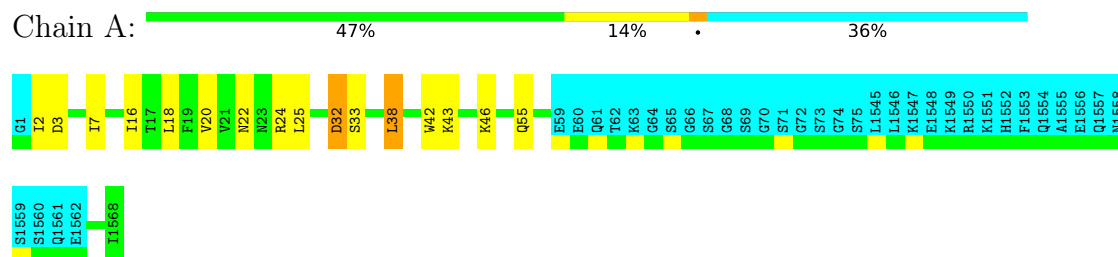
### 4.2.17 Score per residue for model 17

- Molecule 1: NRPS Kj12C-NDD, NRPS Kj12B-CDD



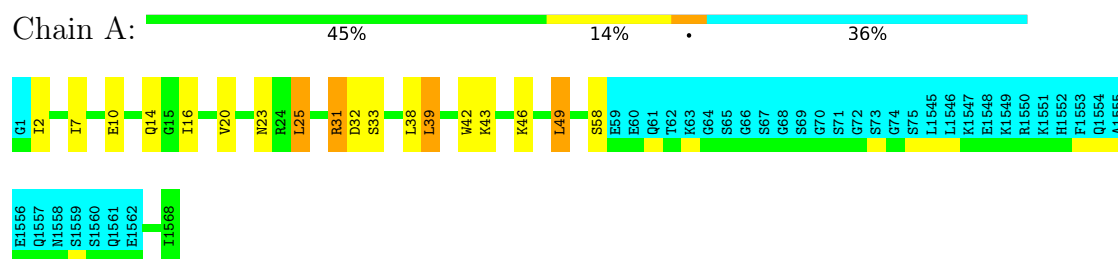
### 4.2.18 Score per residue for model 18

- Molecule 1: NRPS Kj12C-NDD, NRPS Kj12B-CDD



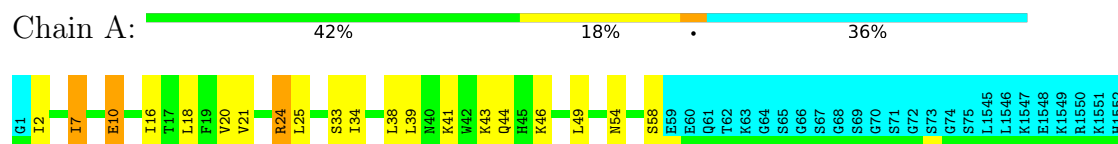
### 4.2.19 Score per residue for model 19

- Molecule 1: NRPS Kj12C-NDD, NRPS Kj12B-CDD



### 4.2.20 Score per residue for model 20

- Molecule 1: NRPS Kj12C-NDD, NRPS Kj12B-CDD



|       |       |
|-------|-------|
| F1553 | I1568 |
| Q1554 |       |
| A1555 |       |
| E1556 |       |
| Q1557 |       |
| M1558 |       |
| S1559 |       |
| S1560 |       |
| Q1561 |       |
| E1562 |       |

## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| OPALp         | refinement            | 3.97    |
| CYANA         | structure calculation | 3.97    |

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                       | 1028           |
| Number of shifts mapped to atoms             | 1028           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 83%            |

## 6 Model quality i

### 6.1 Standard geometry i

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 0.67±0.23    | 0±0/527 ( 0.0± 0.0%) | 1.44±0.09   | 3±2/713 ( 0.4± 0.3%) |
| All | All   | 0.71         | 1/10540 ( 0.0%)      | 1.44        | 60/14260 ( 0.4%)     |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 0.6±0.7   |
| All | All   | 0         | 12        |

All unique bond outliers are listed below.

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|------|------|-------|-------|-------------|----------|--------|-------|
|     |       |      |      |       |       |             |          | Worst  | Total |
| 1   | A     | 1568 | ILE  | C-O   | 38.46 | 2.00        | 1.23     | 2      | 1     |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|------|------|----------|-------|-------------|----------|--------|-------|
|     |       |      |      |          |       |             |          | Worst  | Total |
| 1   | A     | 1568 | ILE  | CA-C-O   | 23.75 | 161.18      | 120.80   | 2      | 1     |
| 1   | A     | 34   | ILE  | CA-C-N   | 7.60  | 127.36      | 119.76   | 10     | 2     |
| 1   | A     | 34   | ILE  | C-N-CA   | 7.60  | 127.36      | 119.76   | 10     | 2     |
| 1   | A     | 32   | ASP  | CA-C-N   | 6.52  | 134.00      | 121.54   | 18     | 12    |
| 1   | A     | 32   | ASP  | C-N-CA   | 6.52  | 134.00      | 121.54   | 18     | 12    |
| 1   | A     | 33   | SER  | CA-C-N   | 6.49  | 127.27      | 122.59   | 16     | 2     |
| 1   | A     | 33   | SER  | C-N-CA   | 6.49  | 127.27      | 122.59   | 16     | 2     |
| 1   | A     | 52   | PHE  | CA-CB-CG | 6.44  | 120.24      | 113.80   | 14     | 2     |
| 1   | A     | 1564 | LEU  | CB-CA-C  | 6.41  | 120.92      | 109.38   | 16     | 2     |
| 1   | A     | 45   | HIS  | CA-C-N   | 5.99  | 128.22      | 120.44   | 13     | 3     |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|------|------|-----------|-------|-------------|----------|--------|-------|
|     |       |      |      |           |       |             |          | Worst  | Total |
| 1   | A     | 45   | HIS  | C-N-CA    | 5.99  | 128.22      | 120.44   | 13     | 3     |
| 1   | A     | 24   | ARG  | CD-NE-CZ  | 5.47  | 132.05      | 124.40   | 9      | 2     |
| 1   | A     | 1568 | ILE  | CA-CB-CG2 | 5.43  | 119.73      | 110.50   | 11     | 4     |
| 1   | A     | 22   | ASN  | CA-C-N    | 5.39  | 130.50      | 122.74   | 18     | 2     |
| 1   | A     | 22   | ASN  | C-N-CA    | 5.39  | 130.50      | 122.74   | 18     | 2     |
| 1   | A     | 9    | ASP  | CA-C-N    | 5.28  | 127.35      | 120.28   | 9      | 1     |
| 1   | A     | 9    | ASP  | C-N-CA    | 5.28  | 127.35      | 120.28   | 9      | 1     |
| 1   | A     | 30   | SER  | CA-C-O    | -5.26 | 115.05      | 121.58   | 10     | 2     |
| 1   | A     | 40   | ASN  | CA-CB-CG  | 5.11  | 117.71      | 112.60   | 6      | 1     |
| 1   | A     | 7    | ILE  | N-CA-C    | -5.09 | 105.54      | 110.42   | 20     | 1     |
| 1   | A     | 45   | HIS  | CB-CG-CD2 | -5.04 | 124.64      | 131.20   | 12     | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res  | Type | Group     | Models (Total) |
|-----|-------|------|------|-----------|----------------|
| 1   | A     | 24   | ARG  | Sidechain | 5              |
| 1   | A     | 1563 | TYR  | Sidechain | 3              |
| 1   | A     | 27   | TYR  | Sidechain | 2              |
| 1   | A     | 31   | ARG  | Sidechain | 2              |

## 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     | 520   | 515      | 515      | 4±5     |
| All | All   | 10400 | 10300    | 10300    | 74      |

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 4.

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

| Atom-1         | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|----------------|----------------|----------|-------------|--------|-------|
|                |                |          |             | Worst  | Total |
| 1:A:1568:ILE:O | 1:A:1568:ILE:C | 1.05     | 2.00        | 2      | 1     |

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| Atom-1            | Atom-2            | Clash(Å) | Distance(Å) | Models |       |
|-------------------|-------------------|----------|-------------|--------|-------|
|                   |                   |          |             | Worst  | Total |
| 1:A:38:LEU:HD13   | 1:A:42:TRP:CZ2    | 0.73     | 2.18        | 11     | 18    |
| 1:A:38:LEU:HD12   | 1:A:39:LEU:N      | 0.72     | 1.99        | 2      | 8     |
| 1:A:38:LEU:HD13   | 1:A:42:TRP:CH2    | 0.68     | 2.24        | 2      | 11    |
| 1:A:7:ILE:HG21    | 1:A:49:LEU:HD11   | 0.63     | 1.70        | 2      | 1     |
| 1:A:18:LEU:HD12   | 1:A:18:LEU:O      | 0.60     | 1.96        | 2      | 1     |
| 1:A:32:ASP:O      | 1:A:33:SER:CB     | 0.59     | 2.51        | 2      | 1     |
| 1:A:16:ILE:HD12   | 1:A:29:THR:HG21   | 0.57     | 1.76        | 2      | 2     |
| 1:A:30:SER:HB3    | 1:A:1563:TYR:CD1  | 0.51     | 2.40        | 2      | 1     |
| 1:A:18:LEU:CD2    | 1:A:42:TRP:CZ2    | 0.50     | 2.95        | 17     | 2     |
| 1:A:46:LYS:HB2    | 1:A:1568:ILE:HG22 | 0.49     | 1.85        | 2      | 1     |
| 1:A:38:LEU:HD12   | 1:A:39:LEU:H      | 0.48     | 1.69        | 2      | 1     |
| 1:A:18:LEU:HD12   | 1:A:18:LEU:C      | 0.48     | 2.33        | 2      | 1     |
| 1:A:1564:LEU:HD12 | 1:A:1564:LEU:O    | 0.47     | 2.09        | 2      | 1     |
| 1:A:30:SER:HB3    | 1:A:1563:TYR:CG   | 0.47     | 2.45        | 2      | 1     |
| 1:A:10:GLU:OE2    | 1:A:41:LYS:HE3    | 0.46     | 2.10        | 1      | 1     |
| 1:A:2:ILE:HD13    | 1:A:3:ASP:N       | 0.46     | 2.25        | 2      | 1     |
| 1:A:25:LEU:HD11   | 1:A:49:LEU:HD13   | 0.46     | 1.86        | 2      | 1     |
| 1:A:46:LYS:CE     | 1:A:50:ILE:HD12   | 0.45     | 2.42        | 2      | 1     |
| 1:A:33:SER:HA     | 1:A:1564:LEU:HD21 | 0.45     | 1.87        | 16     | 3     |
| 1:A:2:ILE:O       | 1:A:2:ILE:CG2     | 0.44     | 2.65        | 2      | 1     |
| 1:A:7:ILE:HG23    | 1:A:41:LYS:HE3    | 0.44     | 1.90        | 17     | 1     |
| 1:A:25:LEU:HB3    | 1:A:1568:ILE:HB   | 0.43     | 1.89        | 2      | 1     |
| 1:A:30:SER:CB     | 1:A:1563:TYR:CD1  | 0.43     | 3.01        | 2      | 1     |
| 1:A:10:GLU:OE1    | 1:A:41:LYS:HE3    | 0.43     | 2.13        | 20     | 1     |
| 1:A:27:TYR:CE1    | 1:A:1566:GLY:HA3  | 0.43     | 2.48        | 12     | 1     |
| 1:A:34:ILE:HG21   | 1:A:39:LEU:HD12   | 0.42     | 1.91        | 20     | 1     |
| 1:A:20:VAL:O      | 1:A:20:VAL:HG12   | 0.42     | 2.14        | 2      | 1     |
| 1:A:7:ILE:CG2     | 1:A:49:LEU:HD11   | 0.42     | 2.42        | 2      | 1     |
| 1:A:20:VAL:HG23   | 1:A:53:LEU:HB2    | 0.41     | 1.91        | 2      | 1     |
| 1:A:25:LEU:HD21   | 1:A:49:LEU:CB     | 0.41     | 2.46        | 19     | 1     |
| 1:A:18:LEU:HD23   | 1:A:42:TRP:CZ2    | 0.41     | 2.51        | 15     | 1     |
| 1:A:27:TYR:CD2    | 1:A:27:TYR:C      | 0.41     | 2.98        | 15     | 1     |
| 1:A:25:LEU:HD21   | 1:A:49:LEU:HB2    | 0.41     | 1.93        | 19     | 1     |
| 1:A:46:LYS:HE2    | 1:A:50:ILE:HD12   | 0.40     | 1.92        | 10     | 1     |
| 1:A:19:PHE:O      | 1:A:25:LEU:HD23   | 0.40     | 2.16        | 2      | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|------------|-------------|----|
| 1   | A     | 62/99 (63%)     | 58±1 (93±1%) | 3±1 (5±1%) | 1±0 (2±0%) | 9           | 53 |
| All | All   | 1240/1980 (63%) | 1151 (93%)   | 68 (5%)    | 21 (2%)    | 9           | 53 |

All 2 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  | SER  | 20             |
| 1   | A     | 2   | ILE  | 1              |

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

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

| Mol | Chain | Analysed        | Rotameric    | Outliers     | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|-------------|----|
| 1   | A     | 58/86 (67%)     | 44±2 (75±3%) | 14±2 (25±3%) | 2           | 25 |
| All | All   | 1160/1720 (67%) | 873 (75%)    | 287 (25%)    | 2           | 25 |

All 36 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     | 2   | ILE  | 20             |
| 1   | A     | 7   | ILE  | 20             |
| 1   | A     | 16  | ILE  | 20             |
| 1   | A     | 43  | LYS  | 20             |
| 1   | A     | 46  | LYS  | 20             |
| 1   | A     | 20  | VAL  | 19             |
| 1   | A     | 49  | LEU  | 17             |
| 1   | A     | 25  | LEU  | 16             |

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| Mol | Chain | Res  | Type | Models (Total) |
|-----|-------|------|------|----------------|
| 1   | A     | 24   | ARG  | 15             |
| 1   | A     | 41   | LYS  | 11             |
| 1   | A     | 58   | SER  | 11             |
| 1   | A     | 3    | ASP  | 10             |
| 1   | A     | 18   | LEU  | 8              |
| 1   | A     | 21   | VAL  | 8              |
| 1   | A     | 23   | ASN  | 7              |
| 1   | A     | 38   | LEU  | 7              |
| 1   | A     | 39   | LEU  | 7              |
| 1   | A     | 9    | ASP  | 6              |
| 1   | A     | 31   | ARG  | 6              |
| 1   | A     | 10   | GLU  | 5              |
| 1   | A     | 28   | GLU  | 4              |
| 1   | A     | 55   | GLN  | 4              |
| 1   | A     | 32   | ASP  | 4              |
| 1   | A     | 33   | SER  | 3              |
| 1   | A     | 52   | PHE  | 3              |
| 1   | A     | 54   | ASN  | 3              |
| 1   | A     | 17   | THR  | 2              |
| 1   | A     | 30   | SER  | 2              |
| 1   | A     | 44   | GLN  | 2              |
| 1   | A     | 1565 | ARG  | 1              |
| 1   | A     | 1564 | LEU  | 1              |
| 1   | A     | 40   | ASN  | 1              |
| 1   | A     | 47   | GLN  | 1              |
| 1   | A     | 13   | GLU  | 1              |
| 1   | A     | 56   | LEU  | 1              |
| 1   | A     | 14   | GLN  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 77% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *komplex.str*

#### 7.1.1 Bookkeeping [i](#)

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                  | 1028 |
| Number of shifts mapped to atoms        | 1028 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 2    |

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 90       | $-0.32 \pm 0.14$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 85       | $0.12 \pm 0.13$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 89       | $-0.29 \pm 0.22$                | 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 83%, i.e. 751 atoms were assigned a chemical shift out of a possible 906. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 250/315 (79%) | 126/127 (99%) | 63/126 (50%)    | 61/62 (98%)     |
| Sidechain | 453/534 (85%) | 309/344 (90%) | 144/168 (86%)   | 0/22 (0%)       |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 48/57 (84%)   | 24/28 (86%)    | 23/27 (85%)     | 1/2 (50%)       |
| Overall  | 751/906 (83%) | 459/499 (92%)  | 230/321 (72%)   | 62/86 (72%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1028 atoms were assigned a chemical shift out of a possible 1328. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 362/502 (72%)   | 183/206 (89%)  | 90/198 (45%)    | 89/98 (91%)     |
| Sidechain | 612/752 (81%)   | 416/480 (87%)  | 196/238 (82%)   | 0/34 (0%)       |
| Aromatic  | 54/74 (73%)     | 27/37 (73%)    | 26/34 (76%)     | 1/3 (33%)       |
| Overall   | 1028/1328 (77%) | 626/723 (87%)  | 312/470 (66%)   | 90/135 (67%)    |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

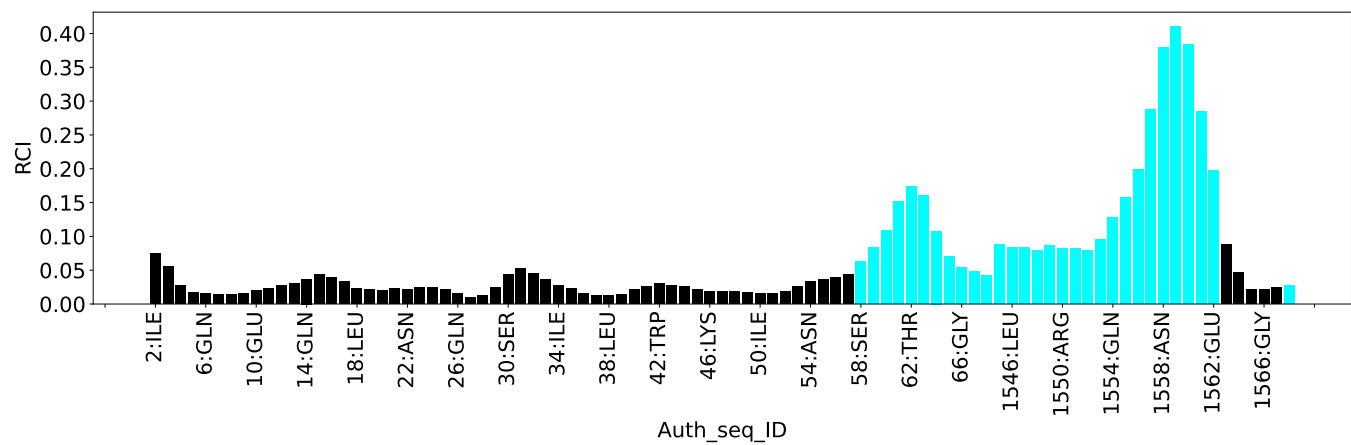
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 31  | ARG  | CG   | 36.31      | 21.24 – 33.19       | 7.6     |
| 1       | A     | 26  | GLN  | HB3  | 0.10       | 0.71 – 3.33         | -7.3    |

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

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

Random coil index (RCI) for chain A:



## 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                                | 2236  |
| Intra-residue ( $ i-j =0$ )                              | 430   |
| Sequential ( $ i-j =1$ )                                 | 584   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 614   |
| Long range ( $ i-j \geq 5$ )                             | 608   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 139   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 24.0  |
| Number of long range restraints per residue <sup>1</sup> | 6.1   |

<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)  | 5.8                                    | 0.18    |
| 0.2-0.5 (Medium) | 0.7                                    | 0.47    |
| >0.5 (Large)     | 0.2                                    | 0.8     |

### 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)   | 15.2                                   | 9.88    |
| 10.0-20.0 (Medium) | 2.2                                    | 19.99   |
| >20.0 (Large)      | 0.1                                    | 34.55   |

## 9 Distance violation analysis ⓘ

### 9.1 Summary of distance violations ⓘ

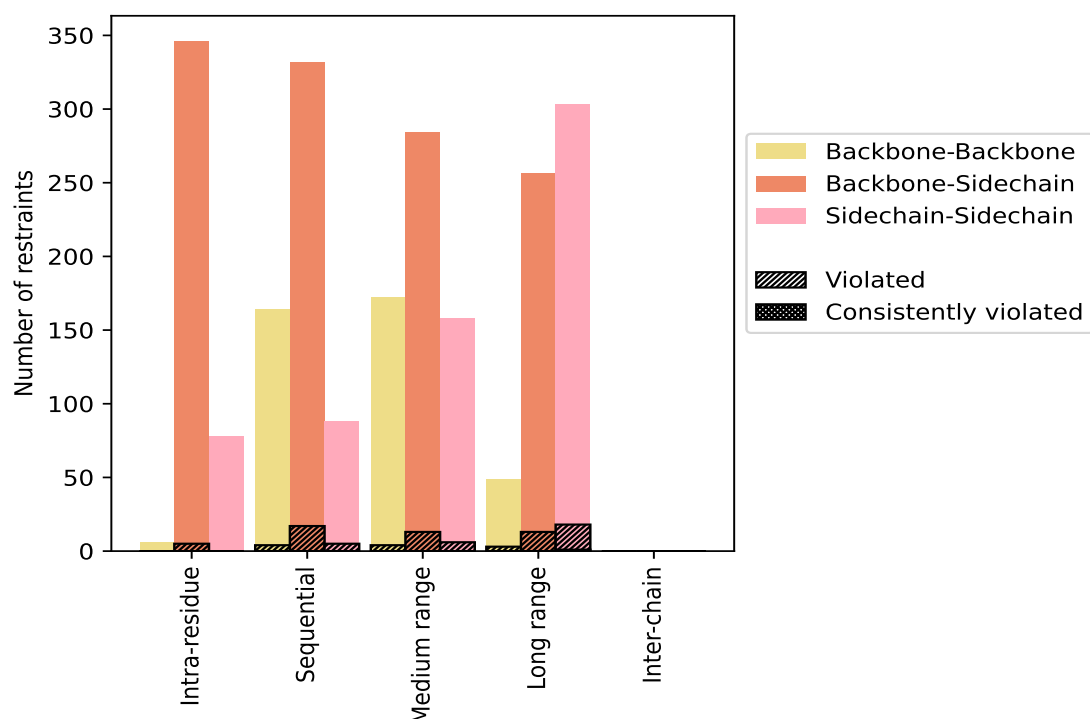
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

| Restrains type                                             | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                     |                     | Consistently Violated <sup>4</sup> |                     |                     |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|---------------------|---------------------|------------------------------------|---------------------|---------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>      | % <sup>1</sup>      | Count                              | % <sup>2</sup>      | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">430</a>  | <a href="#">19.2</a>  | <a href="#">5</a>     | <a href="#">1.2</a> | <a href="#">0.2</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 6                    | 0.3                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 346                  | 15.5                  | 5                     | 1.4                 | 0.2                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 78                   | 3.5                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">584</a>  | <a href="#">26.1</a>  | <a href="#">26</a>    | <a href="#">4.5</a> | <a href="#">1.2</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 164                  | 7.3                   | 4                     | 2.4                 | 0.2                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 332                  | 14.8                  | 17                    | 5.1                 | 0.8                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 88                   | 3.9                   | 5                     | 5.7                 | 0.2                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">614</a>  | <a href="#">27.5</a>  | <a href="#">23</a>    | <a href="#">3.7</a> | <a href="#">1.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 172                  | 7.7                   | 4                     | 2.3                 | 0.2                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 284                  | 12.7                  | 13                    | 4.6                 | 0.6                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 158                  | 7.1                   | 6                     | 3.8                 | 0.3                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">608</a>  | <a href="#">27.2</a>  | <a href="#">34</a>    | <a href="#">5.6</a> | <a href="#">1.5</a> | <a href="#">1</a>                  | <a href="#">0.2</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 49                   | 2.2                   | 3                     | 6.1                 | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 256                  | 11.4                  | 13                    | 5.1                 | 0.6                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 303                  | 13.6                  | 18                    | 5.9                 | 0.8                 | 1                                  | 0.3                 | 0.0                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 0                    | 0.0                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 0                    | 0.0                   | 0                     | 0.0                 | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a> | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">2236</a> | <a href="#">100.0</a> | <a href="#">88</a>    | <a href="#">3.9</a> | <a href="#">3.9</a> | <a href="#">1</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 391                  | 17.5                  | 11                    | 2.8                 | 0.5                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 1218                 | 54.5                  | 48                    | 3.9                 | 2.1                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 627                  | 28.0                  | 29                    | 4.6                 | 1.3                 | 1                                  | 0.2                 | 0.0                 |

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



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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 0                    | 0               | 1               | 3               | 0               | 4     | 0.11     | 0.11    | 0.0                 | 0.11       |
| 2        | 2                    | 16              | 16              | 12              | 0               | 46    | 0.22     | 0.8     | 0.16                | 0.15       |
| 3        | 0                    | 1               | 1               | 7               | 0               | 9     | 0.11     | 0.11    | 0.0                 | 0.11       |
| 4        | 0                    | 1               | 1               | 3               | 0               | 5     | 0.11     | 0.12    | 0.01                | 0.1        |
| 5        | 0                    | 0               | 2               | 7               | 0               | 9     | 0.11     | 0.13    | 0.01                | 0.11       |
| 6        | 0                    | 1               | 1               | 4               | 0               | 6     | 0.1      | 0.11    | 0.0                 | 0.11       |
| 7        | 1                    | 1               | 1               | 5               | 0               | 8     | 0.11     | 0.12    | 0.01                | 0.11       |
| 8        | 1                    | 1               | 2               | 7               | 0               | 11    | 0.11     | 0.15    | 0.01                | 0.11       |
| 9        | 0                    | 1               | 1               | 5               | 0               | 7     | 0.12     | 0.14    | 0.01                | 0.11       |
| 10       | 0                    | 1               | 1               | 6               | 0               | 8     | 0.1      | 0.12    | 0.01                | 0.1        |

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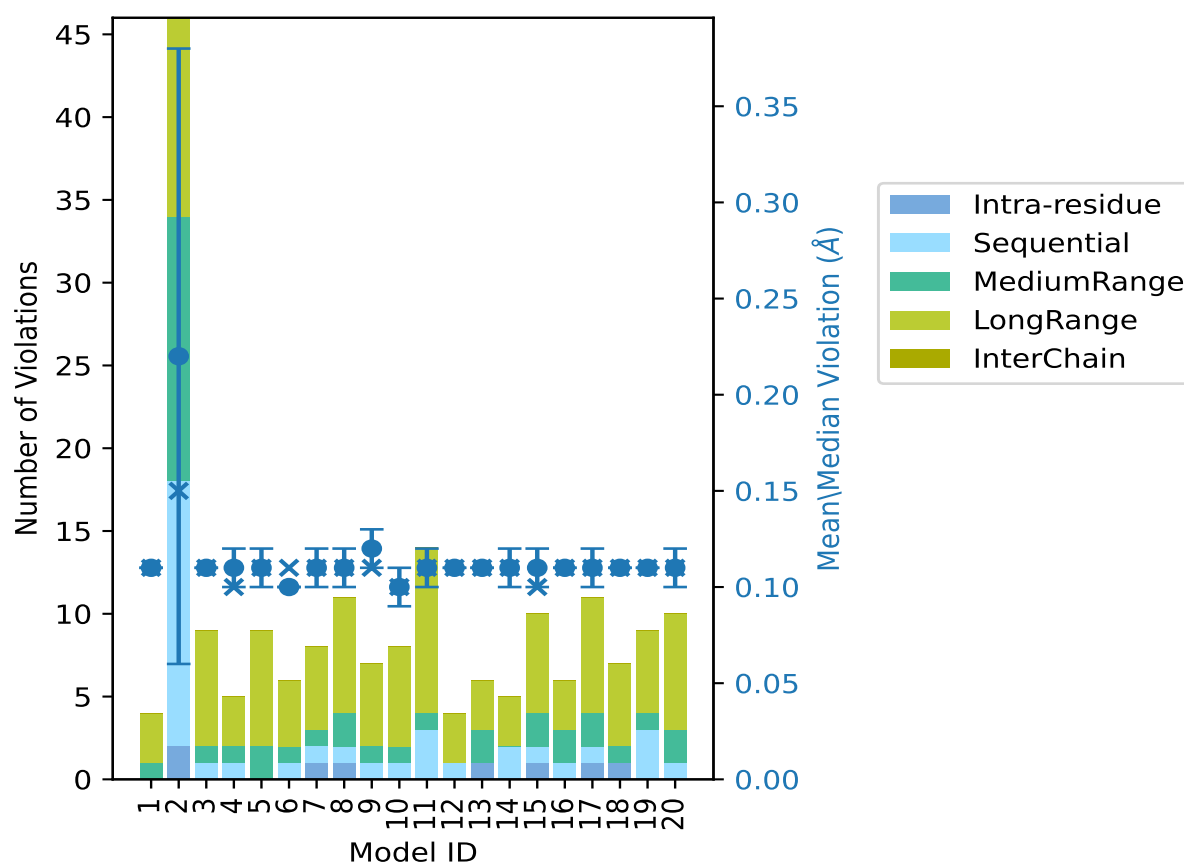
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 0                    | 3               | 1               | 10              | 0               | 14    | 0.11     | 0.12    | 0.01                | 0.11       |
| 12       | 0                    | 1               | 0               | 3               | 0               | 4     | 0.11     | 0.11    | 0.0                 | 0.11       |
| 13       | 1                    | 0               | 2               | 3               | 0               | 6     | 0.11     | 0.11    | 0.0                 | 0.11       |
| 14       | 0                    | 2               | 0               | 3               | 0               | 5     | 0.11     | 0.12    | 0.01                | 0.11       |
| 15       | 1                    | 1               | 2               | 6               | 0               | 10    | 0.11     | 0.12    | 0.01                | 0.1        |
| 16       | 0                    | 1               | 2               | 3               | 0               | 6     | 0.11     | 0.11    | 0.0                 | 0.11       |
| 17       | 1                    | 1               | 2               | 7               | 0               | 11    | 0.11     | 0.12    | 0.01                | 0.11       |
| 18       | 1                    | 0               | 1               | 5               | 0               | 7     | 0.11     | 0.11    | 0.0                 | 0.11       |
| 19       | 0                    | 3               | 1               | 5               | 0               | 9     | 0.11     | 0.11    | 0.0                 | 0.11       |
| 20       | 0                    | 1               | 2               | 7               | 0               | 10    | 0.11     | 0.13    | 0.01                | 0.11       |

<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

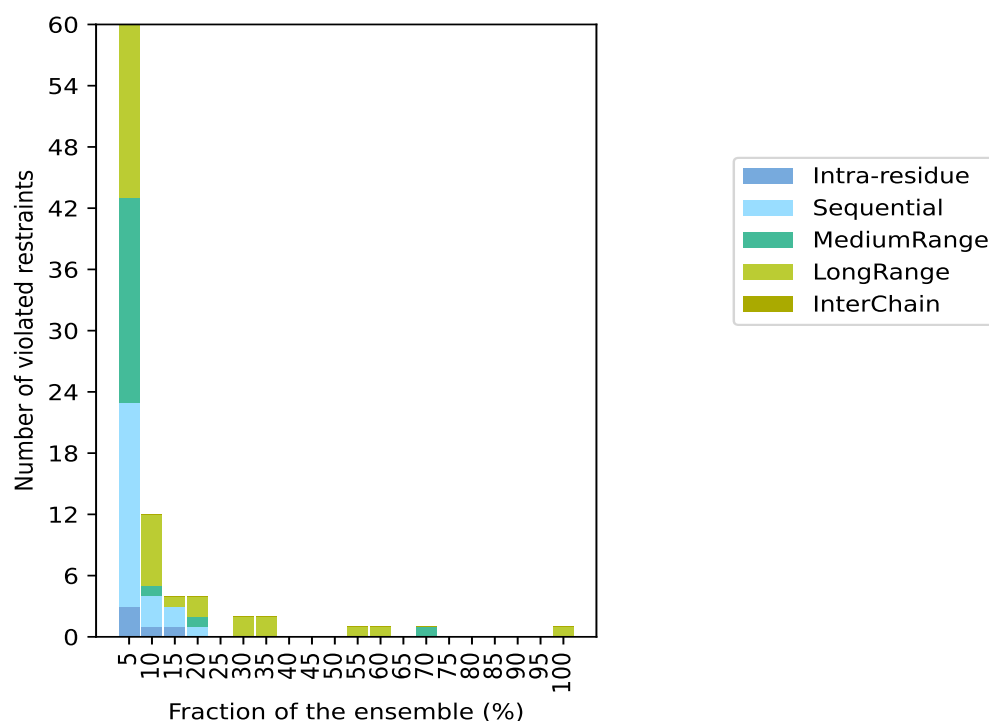
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2148(IR:425, SQ:558, MR:591, LR:574, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 3                             | 20              | 20              | 17              | 0               | 60    | 1                        | 5.0   |
| 1                             | 3               | 1               | 7               | 0               | 12    | 2                        | 10.0  |
| 1                             | 2               | 0               | 1               | 0               | 4     | 3                        | 15.0  |
| 0                             | 1               | 1               | 2               | 0               | 4     | 4                        | 20.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 5                        | 25.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 6                        | 30.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 7                        | 35.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 8                        | 40.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 9                        | 45.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 10                       | 50.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 11                       | 55.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 12                       | 60.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 13                       | 65.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 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  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 19                       | 95.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 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

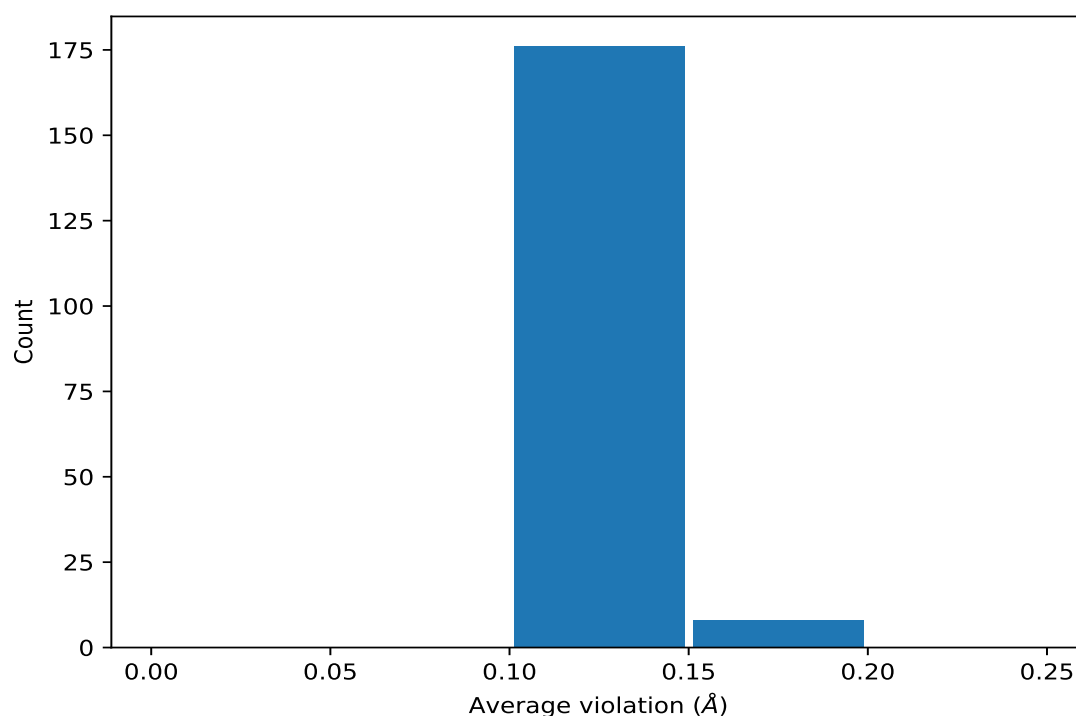
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (1,1782) | 1:42:A:TRP:HE1    | 1:1568:A:ILE:HG21 | 20                  | 0.12     | 0.02                | 0.11       |
| (1,1782) | 1:42:A:TRP:HE1    | 1:1568:A:ILE:HG22 | 20                  | 0.12     | 0.02                | 0.11       |
| (1,1782) | 1:42:A:TRP:HE1    | 1:1568:A:ILE:HG23 | 20                  | 0.12     | 0.02                | 0.11       |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H    | 14                  | 0.11     | 0.01                | 0.11       |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H    | 14                  | 0.11     | 0.01                | 0.11       |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H    | 14                  | 0.11     | 0.01                | 0.11       |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H    | 14                  | 0.11     | 0.01                | 0.11       |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H    | 14                  | 0.11     | 0.01                | 0.11       |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H    | 14                  | 0.11     | 0.01                | 0.11       |
| (1,1359) | 1:7:A:ILE:HG21    | 1:49:A:LEU:HA     | 12                  | 0.11     | 0.01                | 0.11       |
| (1,1359) | 1:7:A:ILE:HG22    | 1:49:A:LEU:HA     | 12                  | 0.11     | 0.01                | 0.11       |
| (1,1359) | 1:7:A:ILE:HG23    | 1:49:A:LEU:HA     | 12                  | 0.11     | 0.01                | 0.11       |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD11 | 11                  | 0.11     | 0.01                | 0.11       |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD12 | 11                  | 0.11     | 0.01                | 0.11       |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD13 | 11                  | 0.11     | 0.01                | 0.11       |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD21 | 11                  | 0.11     | 0.01                | 0.11       |

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| Key      | Atom-1          | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-------------------|---------------------|----------|---------------------|------------|
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD22 | 11                  | 0.11     | 0.01                | 0.11       |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD23 | 11                  | 0.11     | 0.01                | 0.11       |
| (1,1898) | 1:18:A:LEU:HD11 | 1:25:A:LEU:HG     | 7                   | 0.12     | 0.03                | 0.11       |
| (1,1898) | 1:18:A:LEU:HD12 | 1:25:A:LEU:HG     | 7                   | 0.12     | 0.03                | 0.11       |
| (1,1898) | 1:18:A:LEU:HD13 | 1:25:A:LEU:HG     | 7                   | 0.12     | 0.03                | 0.11       |
| (1,1898) | 1:18:A:LEU:HD21 | 1:25:A:LEU:HG     | 7                   | 0.12     | 0.03                | 0.11       |
| (1,1898) | 1:18:A:LEU:HD22 | 1:25:A:LEU:HG     | 7                   | 0.12     | 0.03                | 0.11       |
| (1,1898) | 1:18:A:LEU:HD23 | 1:25:A:LEU:HG     | 7                   | 0.12     | 0.03                | 0.11       |
| (1,1906) | 1:18:A:LEU:HD11 | 1:42:A:TRP:H      | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,1906) | 1:18:A:LEU:HD12 | 1:42:A:TRP:H      | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,1906) | 1:18:A:LEU:HD13 | 1:42:A:TRP:H      | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,1906) | 1:18:A:LEU:HD21 | 1:42:A:TRP:H      | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,1906) | 1:18:A:LEU:HD22 | 1:42:A:TRP:H      | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,1906) | 1:18:A:LEU:HD23 | 1:42:A:TRP:H      | 7                   | 0.11     | 0.0                 | 0.11       |
| (1,1228) | 1:34:A:ILE:HD11 | 1:39:A:LEU:HD21   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1228) | 1:34:A:ILE:HD11 | 1:39:A:LEU:HD22   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1228) | 1:34:A:ILE:HD11 | 1:39:A:LEU:HD23   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1228) | 1:34:A:ILE:HD12 | 1:39:A:LEU:HD21   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1228) | 1:34:A:ILE:HD12 | 1:39:A:LEU:HD22   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1228) | 1:34:A:ILE:HD12 | 1:39:A:LEU:HD23   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1228) | 1:34:A:ILE:HD13 | 1:39:A:LEU:HD21   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1228) | 1:34:A:ILE:HD13 | 1:39:A:LEU:HD22   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1228) | 1:34:A:ILE:HD13 | 1:39:A:LEU:HD23   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1958) | 1:25:A:LEU:HD11 | 1:49:A:LEU:H      | 6                   | 0.1      | 0.0                 | 0.1        |
| (1,1958) | 1:25:A:LEU:HD12 | 1:49:A:LEU:H      | 6                   | 0.1      | 0.0                 | 0.1        |
| (1,1958) | 1:25:A:LEU:HD13 | 1:49:A:LEU:H      | 6                   | 0.1      | 0.0                 | 0.1        |
| (1,1958) | 1:25:A:LEU:HD21 | 1:49:A:LEU:H      | 6                   | 0.1      | 0.0                 | 0.1        |
| (1,1958) | 1:25:A:LEU:HD22 | 1:49:A:LEU:H      | 6                   | 0.1      | 0.0                 | 0.1        |
| (1,1958) | 1:25:A:LEU:HD23 | 1:49:A:LEU:H      | 6                   | 0.1      | 0.0                 | 0.1        |
| (1,1441) | 1:25:A:LEU:HB2  | 1:1568:A:ILE:HD11 | 4                   | 0.14     | 0.07                | 0.11       |
| (1,1441) | 1:25:A:LEU:HB2  | 1:1568:A:ILE:HD12 | 4                   | 0.14     | 0.07                | 0.11       |
| (1,1441) | 1:25:A:LEU:HB2  | 1:1568:A:ILE:HD13 | 4                   | 0.14     | 0.07                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD11   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD12   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD13   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD21   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD22   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD23   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD11   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD12   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD13   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD21   | 4                   | 0.11     | 0.01                | 0.11       |

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| Key      | Atom-1           | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-------------------|---------------------|----------|---------------------|------------|
| (1,1409) | 1:11:A:ALA:HB2   | 1:12:A:LEU:HD22   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB2   | 1:12:A:LEU:HD23   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB3   | 1:12:A:LEU:HD11   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB3   | 1:12:A:LEU:HD12   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB3   | 1:12:A:LEU:HD13   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB3   | 1:12:A:LEU:HD21   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB3   | 1:12:A:LEU:HD22   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1409) | 1:11:A:ALA:HB3   | 1:12:A:LEU:HD23   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1934) | 1:21:A:VAL:H     | 1:25:A:LEU:HD11   | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,1934) | 1:21:A:VAL:H     | 1:25:A:LEU:HD12   | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,1934) | 1:21:A:VAL:H     | 1:25:A:LEU:HD13   | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,1934) | 1:21:A:VAL:H     | 1:25:A:LEU:HD21   | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,1934) | 1:21:A:VAL:H     | 1:25:A:LEU:HD22   | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,1934) | 1:21:A:VAL:H     | 1:25:A:LEU:HD23   | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,2033) | 1:42:A:TRP:HD1   | 1:49:A:LEU:HD11   | 4                   | 0.1      | 0.0                 | 0.11       |
| (1,2033) | 1:42:A:TRP:HD1   | 1:49:A:LEU:HD12   | 4                   | 0.1      | 0.0                 | 0.11       |
| (1,2033) | 1:42:A:TRP:HD1   | 1:49:A:LEU:HD13   | 4                   | 0.1      | 0.0                 | 0.11       |
| (1,2033) | 1:42:A:TRP:HD1   | 1:49:A:LEU:HD21   | 4                   | 0.1      | 0.0                 | 0.11       |
| (1,2033) | 1:42:A:TRP:HD1   | 1:49:A:LEU:HD22   | 4                   | 0.1      | 0.0                 | 0.11       |
| (1,2033) | 1:42:A:TRP:HD1   | 1:49:A:LEU:HD23   | 4                   | 0.1      | 0.0                 | 0.11       |
| (1,1126) | 1:1548:A:GLU:HG2 | 1:1549:A:LYS:HA   | 3                   | 0.17     | 0.09                | 0.1        |
| (1,1126) | 1:1548:A:GLU:HG3 | 1:1549:A:LYS:HA   | 3                   | 0.17     | 0.09                | 0.1        |
| (1,1915) | 1:18:A:LEU:HD11  | 1:1568:A:ILE:HD11 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD11  | 1:1568:A:ILE:HD12 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD11  | 1:1568:A:ILE:HD13 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD12  | 1:1568:A:ILE:HD11 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD12  | 1:1568:A:ILE:HD12 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD12  | 1:1568:A:ILE:HD13 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD13  | 1:1568:A:ILE:HD11 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD13  | 1:1568:A:ILE:HD12 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD13  | 1:1568:A:ILE:HD13 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD21  | 1:1568:A:ILE:HD11 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD21  | 1:1568:A:ILE:HD12 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD21  | 1:1568:A:ILE:HD13 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD22  | 1:1568:A:ILE:HD11 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD22  | 1:1568:A:ILE:HD12 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD22  | 1:1568:A:ILE:HD13 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD23  | 1:1568:A:ILE:HD11 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD23  | 1:1568:A:ILE:HD12 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,1915) | 1:18:A:LEU:HD23  | 1:1568:A:ILE:HD13 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,2141) | 1:1545:A:LEU:HA  | 1:1545:A:LEU:HD11 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2141) | 1:1545:A:LEU:HA  | 1:1545:A:LEU:HD12 | 3                   | 0.11     | 0.0                 | 0.11       |

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| Key      | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD13 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD21 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD22 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD23 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1946) | 1:24:A:ARG:H      | 1:25:A:LEU:HD11   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1946) | 1:24:A:ARG:H      | 1:25:A:LEU:HD12   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1946) | 1:24:A:ARG:H      | 1:25:A:LEU:HD13   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1946) | 1:24:A:ARG:H      | 1:25:A:LEU:HD21   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1946) | 1:24:A:ARG:H      | 1:25:A:LEU:HD22   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1946) | 1:24:A:ARG:H      | 1:25:A:LEU:HD23   | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2223) | 1:1564:A:LEU:HD11 | 1:1565:A:ARG:H    | 2                   | 0.18     | 0.08                | 0.18       |
| (1,2223) | 1:1564:A:LEU:HD12 | 1:1565:A:ARG:H    | 2                   | 0.18     | 0.08                | 0.18       |
| (1,2223) | 1:1564:A:LEU:HD13 | 1:1565:A:ARG:H    | 2                   | 0.18     | 0.08                | 0.18       |
| (1,2223) | 1:1564:A:LEU:HD21 | 1:1565:A:ARG:H    | 2                   | 0.18     | 0.08                | 0.18       |
| (1,2223) | 1:1564:A:LEU:HD22 | 1:1565:A:ARG:H    | 2                   | 0.18     | 0.08                | 0.18       |
| (1,2223) | 1:1564:A:LEU:HD23 | 1:1565:A:ARG:H    | 2                   | 0.18     | 0.08                | 0.18       |
| (1,1363) | 1:26:A:GLN:HA     | 1:1568:A:ILE:HG21 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1363) | 1:26:A:GLN:HA     | 1:1568:A:ILE:HG22 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1363) | 1:26:A:GLN:HA     | 1:1568:A:ILE:HG23 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1886) | 1:17:A:THR:HG21   | 1:18:A:LEU:HD11   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG21   | 1:18:A:LEU:HD12   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG21   | 1:18:A:LEU:HD13   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG21   | 1:18:A:LEU:HD21   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG21   | 1:18:A:LEU:HD22   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG21   | 1:18:A:LEU:HD23   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG22   | 1:18:A:LEU:HD11   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG22   | 1:18:A:LEU:HD12   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG22   | 1:18:A:LEU:HD13   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG22   | 1:18:A:LEU:HD21   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG22   | 1:18:A:LEU:HD22   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG22   | 1:18:A:LEU:HD23   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG23   | 1:18:A:LEU:HD11   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG23   | 1:18:A:LEU:HD12   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG23   | 1:18:A:LEU:HD13   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG23   | 1:18:A:LEU:HD21   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG23   | 1:18:A:LEU:HD22   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1886) | 1:17:A:THR:HG23   | 1:18:A:LEU:HD23   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1888) | 1:18:A:LEU:H      | 1:25:A:LEU:HD11   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1888) | 1:18:A:LEU:H      | 1:25:A:LEU:HD12   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1888) | 1:18:A:LEU:H      | 1:25:A:LEU:HD13   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1888) | 1:18:A:LEU:H      | 1:25:A:LEU:HD21   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1888) | 1:18:A:LEU:H      | 1:25:A:LEU:HD22   | 2                   | 0.11     | 0.0                 | 0.11       |

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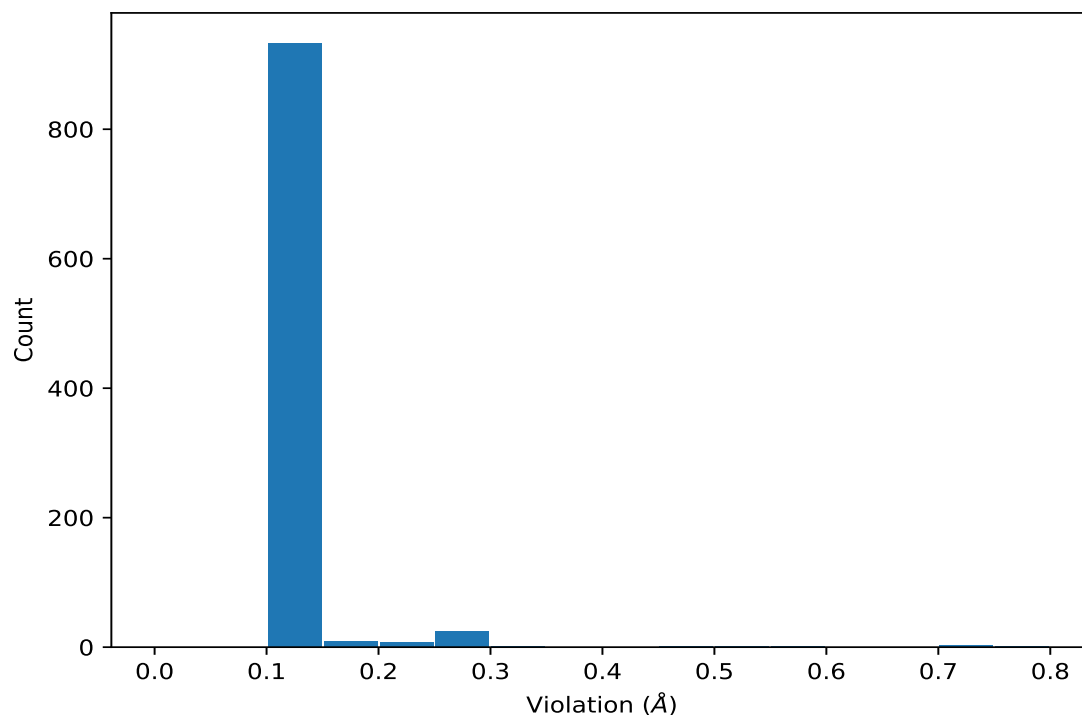
| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1888) | 1:18:A:LEU:H    | 1:25:A:LEU:HD23  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1961) | 1:25:A:LEU:HD11 | 1:49:A:LEU:HG    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1961) | 1:25:A:LEU:HD12 | 1:49:A:LEU:HG    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1961) | 1:25:A:LEU:HD13 | 1:49:A:LEU:HG    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1961) | 1:25:A:LEU:HD21 | 1:49:A:LEU:HG    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1961) | 1:25:A:LEU:HD22 | 1:49:A:LEU:HG    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1961) | 1:25:A:LEU:HD23 | 1:49:A:LEU:HG    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2131) | 1:62:A:THR:HG21 | 1:63:A:LYS:HB2   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2131) | 1:62:A:THR:HG21 | 1:63:A:LYS:HB3   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2131) | 1:62:A:THR:HG22 | 1:63:A:LYS:HB2   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2131) | 1:62:A:THR:HG22 | 1:63:A:LYS:HB3   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2131) | 1:62:A:THR:HG23 | 1:63:A:LYS:HB2   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2131) | 1:62:A:THR:HG23 | 1:63:A:LYS:HB3   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1178) | 1:16:A:ILE:HD11 | 1:35:A:PRO:HG3   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1178) | 1:16:A:ILE:HD12 | 1:35:A:PRO:HG3   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1178) | 1:16:A:ILE:HD13 | 1:35:A:PRO:HG3   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD11  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD12  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD13  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD21  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD22  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD23  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD11  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD12  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD13  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD21  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD22  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD23  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2182) | 1:1550:A:ARG:H  | 1:1550:A:ARG:HG2 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2182) | 1:1550:A:ARG:H  | 1:1550:A:ARG:HG3 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1562) | 1:16:A:ILE:HB   | 1:18:A:LEU:HD11  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1562) | 1:16:A:ILE:HB   | 1:18:A:LEU:HD12  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1562) | 1:16:A:ILE:HB   | 1:18:A:LEU:HD13  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1657) | 1:14:A:GLN:HA   | 1:38:A:LEU:HD21  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1657) | 1:14:A:GLN:HA   | 1:38:A:LEU:HD22  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1657) | 1:14:A:GLN:HA   | 1:38:A:LEU:HD23  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD11  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD12  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD13  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD21  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD22  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD23  | 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) |
|----------|-----------------|------------------|----------|---------------|
| (1,1157) | 1:1549:A:LYS:HA | 1:1552:A:HIS:HB2 | 2        | 0.8           |
| (1,1346) | 1:1552:A:HIS:HA | 1:1555:A:ALA:HB1 | 2        | 0.72          |
| (1,1346) | 1:1552:A:HIS:HA | 1:1555:A:ALA:HB2 | 2        | 0.72          |
| (1,1346) | 1:1552:A:HIS:HA | 1:1555:A:ALA:HB3 | 2        | 0.72          |
| (1,2165) | 1:1547:A:LYS:H  | 1:1550:A:ARG:HB2 | 2        | 0.56          |
| (1,2165) | 1:1547:A:LYS:H  | 1:1550:A:ARG:HB3 | 2        | 0.56          |
| (1,1617) | 1:33:A:SER:HB2  | 1:34:A:ILE:HB    | 2        | 0.53          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,919)  | 1:1556:A:GLU:HA   | 1:1557:A:GLN:H    | 2        | 0.47          |
| (1,385)  | 1:1555:A:ALA:HA   | 1:1556:A:GLU:H    | 2        | 0.34          |
| (1,190)  | 1:1561:A:GLN:HA   | 1:1562:A:GLU:H    | 2        | 0.31          |
| (1,1126) | 1:1548:A:GLU:HG2  | 1:1549:A:LYS:HA   | 2        | 0.3           |
| (1,1126) | 1:1548:A:GLU:HG3  | 1:1549:A:LYS:HA   | 2        | 0.3           |
| (1,344)  | 1:1557:A:GLN:HA   | 1:1558:A:ASN:H    | 2        | 0.3           |
| (1,2207) | 1:1557:A:GLN:HG2  | 1:1559:A:SER:HB2  | 2        | 0.28          |
| (1,2207) | 1:1557:A:GLN:HG2  | 1:1559:A:SER:HB3  | 2        | 0.28          |
| (1,2207) | 1:1557:A:GLN:HG3  | 1:1559:A:SER:HB2  | 2        | 0.28          |
| (1,2207) | 1:1557:A:GLN:HG3  | 1:1559:A:SER:HB3  | 2        | 0.28          |
| (1,2223) | 1:1564:A:LEU:HD11 | 1:1565:A:ARG:H    | 2        | 0.27          |
| (1,2223) | 1:1564:A:LEU:HD12 | 1:1565:A:ARG:H    | 2        | 0.27          |
| (1,2223) | 1:1564:A:LEU:HD13 | 1:1565:A:ARG:H    | 2        | 0.27          |
| (1,2223) | 1:1564:A:LEU:HD21 | 1:1565:A:ARG:H    | 2        | 0.27          |
| (1,2223) | 1:1564:A:LEU:HD22 | 1:1565:A:ARG:H    | 2        | 0.27          |
| (1,2223) | 1:1564:A:LEU:HD23 | 1:1565:A:ARG:H    | 2        | 0.27          |
| (1,1692) | 1:1548:A:GLU:HG2  | 1:1550:A:ARG:H    | 2        | 0.27          |
| (1,1692) | 1:1548:A:GLU:HG3  | 1:1550:A:ARG:H    | 2        | 0.27          |
| (1,1441) | 1:25:A:LEU:HB2    | 1:1568:A:ILE:HD11 | 2        | 0.26          |
| (1,1441) | 1:25:A:LEU:HB2    | 1:1568:A:ILE:HD12 | 2        | 0.26          |
| (1,1441) | 1:25:A:LEU:HB2    | 1:1568:A:ILE:HD13 | 2        | 0.26          |
| (1,2062) | 1:48:A:GLU:H      | 1:49:A:LEU:HD11   | 2        | 0.25          |
| (1,2062) | 1:48:A:GLU:H      | 1:49:A:LEU:HD12   | 2        | 0.25          |
| (1,2062) | 1:48:A:GLU:H      | 1:49:A:LEU:HD13   | 2        | 0.25          |
| (1,2062) | 1:48:A:GLU:H      | 1:49:A:LEU:HD21   | 2        | 0.25          |
| (1,2062) | 1:48:A:GLU:H      | 1:49:A:LEU:HD22   | 2        | 0.25          |
| (1,2062) | 1:48:A:GLU:H      | 1:49:A:LEU:HD23   | 2        | 0.25          |
| (1,669)  | 1:31:A:ARG:HB3    | 1:33:A:SER:H      | 2        | 0.24          |
| (1,1782) | 1:42:A:TRP:HE1    | 1:1568:A:ILE:HG21 | 2        | 0.22          |
| (1,1782) | 1:42:A:TRP:HE1    | 1:1568:A:ILE:HG22 | 2        | 0.22          |
| (1,1782) | 1:42:A:TRP:HE1    | 1:1568:A:ILE:HG23 | 2        | 0.22          |
| (1,751)  | 1:27:A:TYR:HD1    | 1:1567:A:GLU:H    | 2        | 0.22          |
| (1,751)  | 1:27:A:TYR:HD2    | 1:1567:A:GLU:H    | 2        | 0.22          |
| (1,78)   | 1:1564:A:LEU:HB2  | 1:1565:A:ARG:H    | 2        | 0.21          |
| (1,1898) | 1:18:A:LEU:HD11   | 1:25:A:LEU:HG     | 2        | 0.18          |
| (1,1898) | 1:18:A:LEU:HD12   | 1:25:A:LEU:HG     | 2        | 0.18          |
| (1,1898) | 1:18:A:LEU:HD13   | 1:25:A:LEU:HG     | 2        | 0.18          |
| (1,1898) | 1:18:A:LEU:HD21   | 1:25:A:LEU:HG     | 2        | 0.18          |
| (1,1898) | 1:18:A:LEU:HD22   | 1:25:A:LEU:HG     | 2        | 0.18          |
| (1,1898) | 1:18:A:LEU:HD23   | 1:25:A:LEU:HG     | 2        | 0.18          |
| (1,698)  | 1:43:A:LYS:H      | 1:44:A:GLN:HB2    | 2        | 0.16          |
| (1,340)  | 1:60:A:GLU:HB2    | 1:61:A:GLN:H      | 2        | 0.16          |

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| Key      | Atom-1           | Atom-2            | Model ID | Violation (Å) |
|----------|------------------|-------------------|----------|---------------|
| (1,340)  | 1:60:A:GLU:HB3   | 1:61:A:GLN:H      | 2        | 0.16          |
| (1,2145) | 1:1545:A:LEU:HB2 | 1:1548:A:GLU:HG2  | 2        | 0.15          |
| (1,2145) | 1:1545:A:LEU:HB2 | 1:1548:A:GLU:HG3  | 2        | 0.15          |
| (1,2145) | 1:1545:A:LEU:HB3 | 1:1548:A:GLU:HG2  | 2        | 0.15          |
| (1,2145) | 1:1545:A:LEU:HB3 | 1:1548:A:GLU:HG3  | 2        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD11  | 1:1568:A:ILE:HD11 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD11  | 1:1568:A:ILE:HD12 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD11  | 1:1568:A:ILE:HD13 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD12  | 1:1568:A:ILE:HD11 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD12  | 1:1568:A:ILE:HD12 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD12  | 1:1568:A:ILE:HD13 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD13  | 1:1568:A:ILE:HD11 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD13  | 1:1568:A:ILE:HD12 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD13  | 1:1568:A:ILE:HD13 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD21  | 1:1568:A:ILE:HD11 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD21  | 1:1568:A:ILE:HD12 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD21  | 1:1568:A:ILE:HD13 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD22  | 1:1568:A:ILE:HD11 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD22  | 1:1568:A:ILE:HD12 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD22  | 1:1568:A:ILE:HD13 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD23  | 1:1568:A:ILE:HD11 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD23  | 1:1568:A:ILE:HD12 | 8        | 0.15          |
| (1,1915) | 1:18:A:LEU:HD23  | 1:1568:A:ILE:HD13 | 8        | 0.15          |
| (1,1205) | 1:39:A:LEU:HG    | 1:42:A:TRP:HZ3    | 2        | 0.15          |
| (1,621)  | 1:17:A:THR:H     | 1:27:A:TYR:HB3    | 2        | 0.15          |
| (1,587)  | 1:28:A:GLU:HA    | 1:1566:A:GLY:H    | 2        | 0.15          |
| (1,88)   | 1:1555:A:ALA:H   | 1:1555:A:ALA:HB1  | 2        | 0.15          |
| (1,88)   | 1:1555:A:ALA:H   | 1:1555:A:ALA:HB2  | 2        | 0.15          |
| (1,88)   | 1:1555:A:ALA:H   | 1:1555:A:ALA:HB3  | 2        | 0.15          |
| (1,1)    | 1:25:A:LEU:H     | 1:1568:A:ILE:H    | 2        | 0.15          |
| (1,1228) | 1:34:A:ILE:HD11  | 1:39:A:LEU:HD21   | 9        | 0.14          |
| (1,1228) | 1:34:A:ILE:HD11  | 1:39:A:LEU:HD22   | 9        | 0.14          |
| (1,1228) | 1:34:A:ILE:HD11  | 1:39:A:LEU:HD23   | 9        | 0.14          |
| (1,1228) | 1:34:A:ILE:HD12  | 1:39:A:LEU:HD21   | 9        | 0.14          |
| (1,1228) | 1:34:A:ILE:HD12  | 1:39:A:LEU:HD22   | 9        | 0.14          |
| (1,1228) | 1:34:A:ILE:HD12  | 1:39:A:LEU:HD23   | 9        | 0.14          |
| (1,1228) | 1:34:A:ILE:HD13  | 1:39:A:LEU:HD21   | 9        | 0.14          |
| (1,1228) | 1:34:A:ILE:HD13  | 1:39:A:LEU:HD22   | 9        | 0.14          |
| (1,1228) | 1:34:A:ILE:HD13  | 1:39:A:LEU:HD23   | 9        | 0.14          |
| (1,986)  | 1:3:A:ASP:HA     | 1:7:A:ILE:HG12    | 2        | 0.14          |
| (1,393)  | 1:38:A:LEU:H     | 1:40:A:ASN:HB3    | 2        | 0.14          |
| (1,345)  | 1:1557:A:GLN:HB3 | 1:1558:A:ASN:H    | 2        | 0.14          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD11 | 9        | 0.13          |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD12 | 9        | 0.13          |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD13 | 9        | 0.13          |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD21 | 9        | 0.13          |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD22 | 9        | 0.13          |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD23 | 9        | 0.13          |
| (1,1978) | 1:26:A:GLN:HG2    | 1:27:A:TYR:H      | 2        | 0.13          |
| (1,1978) | 1:26:A:GLN:HG3    | 1:27:A:TYR:H      | 2        | 0.13          |
| (1,1898) | 1:18:A:LEU:HD11   | 1:25:A:LEU:HG     | 5        | 0.13          |
| (1,1898) | 1:18:A:LEU:HD12   | 1:25:A:LEU:HG     | 5        | 0.13          |
| (1,1898) | 1:18:A:LEU:HD13   | 1:25:A:LEU:HG     | 5        | 0.13          |
| (1,1898) | 1:18:A:LEU:HD21   | 1:25:A:LEU:HG     | 5        | 0.13          |
| (1,1898) | 1:18:A:LEU:HD22   | 1:25:A:LEU:HG     | 5        | 0.13          |
| (1,1898) | 1:18:A:LEU:HD23   | 1:25:A:LEU:HG     | 5        | 0.13          |
| (1,1363) | 1:26:A:GLN:HA     | 1:1568:A:ILE:HG21 | 2        | 0.13          |
| (1,1363) | 1:26:A:GLN:HA     | 1:1568:A:ILE:HG22 | 2        | 0.13          |
| (1,1363) | 1:26:A:GLN:HA     | 1:1568:A:ILE:HG23 | 2        | 0.13          |
| (1,1300) | 1:8:A:VAL:HG11    | 1:11:A:ALA:HA     | 2        | 0.13          |
| (1,1300) | 1:8:A:VAL:HG12    | 1:11:A:ALA:HA     | 2        | 0.13          |
| (1,1300) | 1:8:A:VAL:HG13    | 1:11:A:ALA:HA     | 2        | 0.13          |
| (1,1228) | 1:34:A:ILE:HD11   | 1:39:A:LEU:HD21   | 20       | 0.13          |
| (1,1228) | 1:34:A:ILE:HD11   | 1:39:A:LEU:HD22   | 20       | 0.13          |
| (1,1228) | 1:34:A:ILE:HD11   | 1:39:A:LEU:HD23   | 20       | 0.13          |
| (1,1228) | 1:34:A:ILE:HD12   | 1:39:A:LEU:HD21   | 20       | 0.13          |
| (1,1228) | 1:34:A:ILE:HD12   | 1:39:A:LEU:HD22   | 20       | 0.13          |
| (1,1228) | 1:34:A:ILE:HD12   | 1:39:A:LEU:HD23   | 20       | 0.13          |
| (1,1228) | 1:34:A:ILE:HD13   | 1:39:A:LEU:HD21   | 20       | 0.13          |
| (1,1228) | 1:34:A:ILE:HD13   | 1:39:A:LEU:HD22   | 20       | 0.13          |
| (1,1228) | 1:34:A:ILE:HD13   | 1:39:A:LEU:HD23   | 20       | 0.13          |
| (1,463)  | 1:45:A:HIS:H      | 1:47:A:GLN:H      | 2        | 0.13          |
| (1,457)  | 1:27:A:TYR:H      | 1:1567:A:GLU:H    | 2        | 0.13          |
| (1,218)  | 1:52:A:PHE:HA     | 1:56:A:LEU:H      | 2        | 0.13          |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H    | 2        | 0.12          |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H    | 2        | 0.12          |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H    | 2        | 0.12          |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H    | 2        | 0.12          |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H    | 2        | 0.12          |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H    | 2        | 0.12          |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H    | 9        | 0.12          |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H    | 9        | 0.12          |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H    | 9        | 0.12          |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H    | 9        | 0.12          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H    | 9        | 0.12          |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H    | 9        | 0.12          |
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD11 | 8        | 0.12          |
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD12 | 8        | 0.12          |
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD13 | 8        | 0.12          |
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD21 | 8        | 0.12          |
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD22 | 8        | 0.12          |
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD23 | 8        | 0.12          |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD11 | 8        | 0.12          |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD12 | 8        | 0.12          |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD13 | 8        | 0.12          |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD21 | 8        | 0.12          |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD22 | 8        | 0.12          |
| (1,1996) | 1:32:A:ASP:HA     | 1:1564:A:LEU:HD23 | 8        | 0.12          |
| (1,1915) | 1:18:A:LEU:HD11   | 1:1568:A:ILE:HD11 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD11   | 1:1568:A:ILE:HD12 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD11   | 1:1568:A:ILE:HD13 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD12   | 1:1568:A:ILE:HD11 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD12   | 1:1568:A:ILE:HD12 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD12   | 1:1568:A:ILE:HD13 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD13   | 1:1568:A:ILE:HD11 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD13   | 1:1568:A:ILE:HD12 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD13   | 1:1568:A:ILE:HD13 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD21   | 1:1568:A:ILE:HD11 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD21   | 1:1568:A:ILE:HD12 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD21   | 1:1568:A:ILE:HD13 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD22   | 1:1568:A:ILE:HD11 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD22   | 1:1568:A:ILE:HD12 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD22   | 1:1568:A:ILE:HD13 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD23   | 1:1568:A:ILE:HD11 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD23   | 1:1568:A:ILE:HD12 | 11       | 0.12          |
| (1,1915) | 1:18:A:LEU:HD23   | 1:1568:A:ILE:HD13 | 11       | 0.12          |
| (1,1886) | 1:17:A:THR:HG21   | 1:18:A:LEU:HD11   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG21   | 1:18:A:LEU:HD12   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG21   | 1:18:A:LEU:HD13   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG21   | 1:18:A:LEU:HD21   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG21   | 1:18:A:LEU:HD22   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG21   | 1:18:A:LEU:HD23   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG22   | 1:18:A:LEU:HD11   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG22   | 1:18:A:LEU:HD12   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG22   | 1:18:A:LEU:HD13   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG22   | 1:18:A:LEU:HD21   | 7        | 0.12          |

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| Key      | Atom-1          | Atom-2            | Model ID | Violation (Å) |
|----------|-----------------|-------------------|----------|---------------|
| (1,1886) | 1:17:A:THR:HG22 | 1:18:A:LEU:HD22   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG22 | 1:18:A:LEU:HD23   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG23 | 1:18:A:LEU:HD11   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG23 | 1:18:A:LEU:HD12   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG23 | 1:18:A:LEU:HD13   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG23 | 1:18:A:LEU:HD21   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG23 | 1:18:A:LEU:HD22   | 7        | 0.12          |
| (1,1886) | 1:17:A:THR:HG23 | 1:18:A:LEU:HD23   | 7        | 0.12          |
| (1,1838) | 1:7:A:ILE:HG21  | 1:18:A:LEU:HD11   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG21  | 1:18:A:LEU:HD12   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG21  | 1:18:A:LEU:HD13   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG21  | 1:18:A:LEU:HD21   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG21  | 1:18:A:LEU:HD22   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG21  | 1:18:A:LEU:HD23   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG22  | 1:18:A:LEU:HD11   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG22  | 1:18:A:LEU:HD12   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG22  | 1:18:A:LEU:HD13   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG22  | 1:18:A:LEU:HD21   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG22  | 1:18:A:LEU:HD22   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG22  | 1:18:A:LEU:HD23   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG23  | 1:18:A:LEU:HD11   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG23  | 1:18:A:LEU:HD12   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG23  | 1:18:A:LEU:HD13   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG23  | 1:18:A:LEU:HD21   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG23  | 1:18:A:LEU:HD22   | 17       | 0.12          |
| (1,1838) | 1:7:A:ILE:HG23  | 1:18:A:LEU:HD23   | 17       | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG21 | 5        | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG22 | 5        | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG23 | 5        | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG21 | 10       | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG22 | 10       | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG23 | 10       | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG21 | 11       | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG22 | 11       | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG23 | 11       | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG21 | 15       | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG22 | 15       | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG23 | 15       | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG21 | 20       | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG22 | 20       | 0.12          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG23 | 20       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD11   | 14       | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD12  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD13  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD21  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD22  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD23  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD11  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD12  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD13  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD21  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD22  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD23  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB3  | 1:12:A:LEU:HD11  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB3  | 1:12:A:LEU:HD12  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB3  | 1:12:A:LEU:HD13  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB3  | 1:12:A:LEU:HD21  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB3  | 1:12:A:LEU:HD22  | 14       | 0.12          |
| (1,1409) | 1:11:A:ALA:HB3  | 1:12:A:LEU:HD23  | 14       | 0.12          |
| (1,1359) | 1:7:A:ILE:HG21  | 1:49:A:LEU:HA    | 11       | 0.12          |
| (1,1359) | 1:7:A:ILE:HG22  | 1:49:A:LEU:HA    | 11       | 0.12          |
| (1,1359) | 1:7:A:ILE:HG23  | 1:49:A:LEU:HA    | 11       | 0.12          |
| (1,1228) | 1:34:A:ILE:HD11 | 1:39:A:LEU:HD21  | 4        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD11 | 1:39:A:LEU:HD22  | 4        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD11 | 1:39:A:LEU:HD23  | 4        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD12 | 1:39:A:LEU:HD21  | 4        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD12 | 1:39:A:LEU:HD22  | 4        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD12 | 1:39:A:LEU:HD23  | 4        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD13 | 1:39:A:LEU:HD21  | 4        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD13 | 1:39:A:LEU:HD22  | 4        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD13 | 1:39:A:LEU:HD23  | 4        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD11 | 1:39:A:LEU:HD21  | 5        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD11 | 1:39:A:LEU:HD22  | 5        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD11 | 1:39:A:LEU:HD23  | 5        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD12 | 1:39:A:LEU:HD21  | 5        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD12 | 1:39:A:LEU:HD22  | 5        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD12 | 1:39:A:LEU:HD23  | 5        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD13 | 1:39:A:LEU:HD21  | 5        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD13 | 1:39:A:LEU:HD22  | 5        | 0.12          |
| (1,1228) | 1:34:A:ILE:HD13 | 1:39:A:LEU:HD23  | 5        | 0.12          |
| (1,737)  | 1:1562:A:GLU:H  | 1:1563:A:TYR:HE1 | 2        | 0.12          |
| (1,737)  | 1:1562:A:GLU:H  | 1:1563:A:TYR:HE2 | 2        | 0.12          |
| (1,423)  | 1:43:A:LYS:HB2  | 1:44:A:GLN:H     | 2        | 0.12          |
| (1,247)  | 1:58:A:SER:HA   | 1:60:A:GLU:H     | 2        | 0.12          |

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| Key      | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H    | 1        | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H    | 1        | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H    | 1        | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H    | 1        | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H    | 1        | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H    | 1        | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H    | 13       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H    | 13       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H    | 13       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H    | 13       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H    | 13       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H    | 13       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H    | 16       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H    | 16       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H    | 16       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H    | 16       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H    | 16       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H    | 16       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H    | 17       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H    | 17       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H    | 17       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H    | 17       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H    | 17       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H    | 17       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H    | 18       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H    | 18       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H    | 18       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H    | 18       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H    | 18       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H    | 18       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H    | 20       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H    | 20       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H    | 20       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H    | 20       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H    | 20       | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H    | 20       | 0.11          |
| (1,2182) | 1:1550:A:ARG:H    | 1:1550:A:ARG:HG2  | 15       | 0.11          |
| (1,2182) | 1:1550:A:ARG:H    | 1:1550:A:ARG:HG3  | 15       | 0.11          |
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD11 | 13       | 0.11          |
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD12 | 13       | 0.11          |
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD13 | 13       | 0.11          |
| (1,2141) | 1:1545:A:LEU:HA   | 1:1545:A:LEU:HD21 | 13       | 0.11          |

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| Key      | Atom-1          | Atom-2            | Model ID | Violation (Å) |
|----------|-----------------|-------------------|----------|---------------|
| (1,2141) | 1:1545:A:LEU:HA | 1:1545:A:LEU:HD22 | 13       | 0.11          |
| (1,2141) | 1:1545:A:LEU:HA | 1:1545:A:LEU:HD23 | 13       | 0.11          |
| (1,2141) | 1:1545:A:LEU:HA | 1:1545:A:LEU:HD11 | 18       | 0.11          |
| (1,2141) | 1:1545:A:LEU:HA | 1:1545:A:LEU:HD12 | 18       | 0.11          |
| (1,2141) | 1:1545:A:LEU:HA | 1:1545:A:LEU:HD13 | 18       | 0.11          |
| (1,2141) | 1:1545:A:LEU:HA | 1:1545:A:LEU:HD21 | 18       | 0.11          |
| (1,2141) | 1:1545:A:LEU:HA | 1:1545:A:LEU:HD22 | 18       | 0.11          |
| (1,2141) | 1:1545:A:LEU:HA | 1:1545:A:LEU:HD23 | 18       | 0.11          |
| (1,2131) | 1:62:A:THR:HG21 | 1:63:A:LYS:HB2    | 11       | 0.11          |
| (1,2131) | 1:62:A:THR:HG21 | 1:63:A:LYS:HB3    | 11       | 0.11          |
| (1,2131) | 1:62:A:THR:HG22 | 1:63:A:LYS:HB2    | 11       | 0.11          |
| (1,2131) | 1:62:A:THR:HG22 | 1:63:A:LYS:HB3    | 11       | 0.11          |
| (1,2131) | 1:62:A:THR:HG23 | 1:63:A:LYS:HB2    | 11       | 0.11          |
| (1,2131) | 1:62:A:THR:HG23 | 1:63:A:LYS:HB3    | 11       | 0.11          |
| (1,2131) | 1:62:A:THR:HG21 | 1:63:A:LYS:HB2    | 15       | 0.11          |
| (1,2131) | 1:62:A:THR:HG21 | 1:63:A:LYS:HB3    | 15       | 0.11          |
| (1,2131) | 1:62:A:THR:HG22 | 1:63:A:LYS:HB2    | 15       | 0.11          |
| (1,2131) | 1:62:A:THR:HG22 | 1:63:A:LYS:HB3    | 15       | 0.11          |
| (1,2131) | 1:62:A:THR:HG23 | 1:63:A:LYS:HB2    | 15       | 0.11          |
| (1,2131) | 1:62:A:THR:HG23 | 1:63:A:LYS:HB3    | 15       | 0.11          |
| (1,2084) | 1:51:A:ASP:H    | 1:53:A:LEU:HD11   | 5        | 0.11          |
| (1,2084) | 1:51:A:ASP:H    | 1:53:A:LEU:HD12   | 5        | 0.11          |
| (1,2084) | 1:51:A:ASP:H    | 1:53:A:LEU:HD13   | 5        | 0.11          |
| (1,2084) | 1:51:A:ASP:H    | 1:53:A:LEU:HD21   | 5        | 0.11          |
| (1,2084) | 1:51:A:ASP:H    | 1:53:A:LEU:HD22   | 5        | 0.11          |
| (1,2084) | 1:51:A:ASP:H    | 1:53:A:LEU:HD23   | 5        | 0.11          |
| (1,2033) | 1:42:A:TRP:HD1  | 1:49:A:LEU:HD11   | 18       | 0.11          |
| (1,2033) | 1:42:A:TRP:HD1  | 1:49:A:LEU:HD12   | 18       | 0.11          |
| (1,2033) | 1:42:A:TRP:HD1  | 1:49:A:LEU:HD13   | 18       | 0.11          |
| (1,2033) | 1:42:A:TRP:HD1  | 1:49:A:LEU:HD21   | 18       | 0.11          |
| (1,2033) | 1:42:A:TRP:HD1  | 1:49:A:LEU:HD22   | 18       | 0.11          |
| (1,2033) | 1:42:A:TRP:HD1  | 1:49:A:LEU:HD23   | 18       | 0.11          |
| (1,2033) | 1:42:A:TRP:HD1  | 1:49:A:LEU:HD11   | 20       | 0.11          |
| (1,2033) | 1:42:A:TRP:HD1  | 1:49:A:LEU:HD12   | 20       | 0.11          |
| (1,2033) | 1:42:A:TRP:HD1  | 1:49:A:LEU:HD13   | 20       | 0.11          |
| (1,2033) | 1:42:A:TRP:HD1  | 1:49:A:LEU:HD21   | 20       | 0.11          |
| (1,2033) | 1:42:A:TRP:HD1  | 1:49:A:LEU:HD22   | 20       | 0.11          |
| (1,2033) | 1:42:A:TRP:HD1  | 1:49:A:LEU:HD23   | 20       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD11 | 6        | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD12 | 6        | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD13 | 6        | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD21 | 6        | 0.11          |

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| Key      | Atom-1          | Atom-2            | Model ID | Violation (Å) |
|----------|-----------------|-------------------|----------|---------------|
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD22 | 6        | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD23 | 6        | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD11 | 7        | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD12 | 7        | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD13 | 7        | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD21 | 7        | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD22 | 7        | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD23 | 7        | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD11 | 13       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD12 | 13       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD13 | 13       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD21 | 13       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD22 | 13       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD23 | 13       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD11 | 16       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD12 | 16       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD13 | 16       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD21 | 16       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD22 | 16       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD23 | 16       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD11 | 18       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD12 | 18       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD13 | 18       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD21 | 18       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD22 | 18       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD23 | 18       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD11 | 19       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD12 | 19       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD13 | 19       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD21 | 19       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD22 | 19       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD23 | 19       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD11 | 20       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD12 | 20       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD13 | 20       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD21 | 20       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD22 | 20       | 0.11          |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD23 | 20       | 0.11          |
| (1,1961) | 1:25:A:LEU:HD11 | 1:49:A:LEU:HG     | 3        | 0.11          |
| (1,1961) | 1:25:A:LEU:HD12 | 1:49:A:LEU:HG     | 3        | 0.11          |
| (1,1961) | 1:25:A:LEU:HD13 | 1:49:A:LEU:HG     | 3        | 0.11          |
| (1,1961) | 1:25:A:LEU:HD21 | 1:49:A:LEU:HG     | 3        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1961) | 1:25:A:LEU:HD22 | 1:49:A:LEU:HG   | 3        | 0.11          |
| (1,1961) | 1:25:A:LEU:HD23 | 1:49:A:LEU:HG   | 3        | 0.11          |
| (1,1961) | 1:25:A:LEU:HD11 | 1:49:A:LEU:HG   | 11       | 0.11          |
| (1,1961) | 1:25:A:LEU:HD12 | 1:49:A:LEU:HG   | 11       | 0.11          |
| (1,1961) | 1:25:A:LEU:HD13 | 1:49:A:LEU:HG   | 11       | 0.11          |
| (1,1961) | 1:25:A:LEU:HD21 | 1:49:A:LEU:HG   | 11       | 0.11          |
| (1,1961) | 1:25:A:LEU:HD22 | 1:49:A:LEU:HG   | 11       | 0.11          |
| (1,1961) | 1:25:A:LEU:HD23 | 1:49:A:LEU:HG   | 11       | 0.11          |
| (1,1958) | 1:25:A:LEU:HD11 | 1:49:A:LEU:H    | 18       | 0.11          |
| (1,1958) | 1:25:A:LEU:HD12 | 1:49:A:LEU:H    | 18       | 0.11          |
| (1,1958) | 1:25:A:LEU:HD13 | 1:49:A:LEU:H    | 18       | 0.11          |
| (1,1958) | 1:25:A:LEU:HD21 | 1:49:A:LEU:H    | 18       | 0.11          |
| (1,1958) | 1:25:A:LEU:HD22 | 1:49:A:LEU:H    | 18       | 0.11          |
| (1,1958) | 1:25:A:LEU:HD23 | 1:49:A:LEU:H    | 18       | 0.11          |
| (1,1951) | 1:25:A:LEU:HB3  | 1:53:A:LEU:HD11 | 19       | 0.11          |
| (1,1951) | 1:25:A:LEU:HB3  | 1:53:A:LEU:HD12 | 19       | 0.11          |
| (1,1951) | 1:25:A:LEU:HB3  | 1:53:A:LEU:HD13 | 19       | 0.11          |
| (1,1951) | 1:25:A:LEU:HB3  | 1:53:A:LEU:HD21 | 19       | 0.11          |
| (1,1951) | 1:25:A:LEU:HB3  | 1:53:A:LEU:HD22 | 19       | 0.11          |
| (1,1951) | 1:25:A:LEU:HB3  | 1:53:A:LEU:HD23 | 19       | 0.11          |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD11 | 10       | 0.11          |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD12 | 10       | 0.11          |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD13 | 10       | 0.11          |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD21 | 10       | 0.11          |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD22 | 10       | 0.11          |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD23 | 10       | 0.11          |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD11 | 12       | 0.11          |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD12 | 12       | 0.11          |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD13 | 12       | 0.11          |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD21 | 12       | 0.11          |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD22 | 12       | 0.11          |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD23 | 12       | 0.11          |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD11 | 5        | 0.11          |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD12 | 5        | 0.11          |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD13 | 5        | 0.11          |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD21 | 5        | 0.11          |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD22 | 5        | 0.11          |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD23 | 5        | 0.11          |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD11 | 20       | 0.11          |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD12 | 20       | 0.11          |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD13 | 20       | 0.11          |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD21 | 20       | 0.11          |

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| Key      | Atom-1          | Atom-2            | Model ID | Violation (Å) |
|----------|-----------------|-------------------|----------|---------------|
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD22   | 20       | 0.11          |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD23   | 20       | 0.11          |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD11   | 12       | 0.11          |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD12   | 12       | 0.11          |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD13   | 12       | 0.11          |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD21   | 12       | 0.11          |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD22   | 12       | 0.11          |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD23   | 12       | 0.11          |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD11   | 12       | 0.11          |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD12   | 12       | 0.11          |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD13   | 12       | 0.11          |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD21   | 12       | 0.11          |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD22   | 12       | 0.11          |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD23   | 12       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD11 | 1:1568:A:ILE:HD11 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD11 | 1:1568:A:ILE:HD12 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD11 | 1:1568:A:ILE:HD13 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD12 | 1:1568:A:ILE:HD11 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD12 | 1:1568:A:ILE:HD12 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD12 | 1:1568:A:ILE:HD13 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD13 | 1:1568:A:ILE:HD11 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD13 | 1:1568:A:ILE:HD12 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD13 | 1:1568:A:ILE:HD13 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD21 | 1:1568:A:ILE:HD11 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD21 | 1:1568:A:ILE:HD12 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD21 | 1:1568:A:ILE:HD13 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD22 | 1:1568:A:ILE:HD11 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD22 | 1:1568:A:ILE:HD12 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD22 | 1:1568:A:ILE:HD13 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD23 | 1:1568:A:ILE:HD11 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD23 | 1:1568:A:ILE:HD12 | 17       | 0.11          |
| (1,1915) | 1:18:A:LEU:HD23 | 1:1568:A:ILE:HD13 | 17       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD11 | 1:42:A:TRP:H      | 2        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD12 | 1:42:A:TRP:H      | 2        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD13 | 1:42:A:TRP:H      | 2        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD21 | 1:42:A:TRP:H      | 2        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD22 | 1:42:A:TRP:H      | 2        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD23 | 1:42:A:TRP:H      | 2        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD11 | 1:42:A:TRP:H      | 3        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD12 | 1:42:A:TRP:H      | 3        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD13 | 1:42:A:TRP:H      | 3        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD21 | 1:42:A:TRP:H      | 3        | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1906) | 1:18:A:LEU:HD22 | 1:42:A:TRP:H   | 3        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD23 | 1:42:A:TRP:H   | 3        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD11 | 1:42:A:TRP:H   | 8        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD12 | 1:42:A:TRP:H   | 8        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD13 | 1:42:A:TRP:H   | 8        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD21 | 1:42:A:TRP:H   | 8        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD22 | 1:42:A:TRP:H   | 8        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD23 | 1:42:A:TRP:H   | 8        | 0.11          |
| (1,1906) | 1:18:A:LEU:HD11 | 1:42:A:TRP:H   | 11       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD12 | 1:42:A:TRP:H   | 11       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD13 | 1:42:A:TRP:H   | 11       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD21 | 1:42:A:TRP:H   | 11       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD22 | 1:42:A:TRP:H   | 11       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD23 | 1:42:A:TRP:H   | 11       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD11 | 1:42:A:TRP:H   | 17       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD12 | 1:42:A:TRP:H   | 17       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD13 | 1:42:A:TRP:H   | 17       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD21 | 1:42:A:TRP:H   | 17       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD22 | 1:42:A:TRP:H   | 17       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD23 | 1:42:A:TRP:H   | 17       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD11 | 1:42:A:TRP:H   | 20       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD12 | 1:42:A:TRP:H   | 20       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD13 | 1:42:A:TRP:H   | 20       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD21 | 1:42:A:TRP:H   | 20       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD22 | 1:42:A:TRP:H   | 20       | 0.11          |
| (1,1906) | 1:18:A:LEU:HD23 | 1:42:A:TRP:H   | 20       | 0.11          |
| (1,1905) | 1:18:A:LEU:HD11 | 1:27:A:TYR:HD1 | 11       | 0.11          |
| (1,1905) | 1:18:A:LEU:HD11 | 1:27:A:TYR:HD2 | 11       | 0.11          |
| (1,1905) | 1:18:A:LEU:HD12 | 1:27:A:TYR:HD1 | 11       | 0.11          |
| (1,1905) | 1:18:A:LEU:HD12 | 1:27:A:TYR:HD2 | 11       | 0.11          |
| (1,1905) | 1:18:A:LEU:HD13 | 1:27:A:TYR:HD1 | 11       | 0.11          |
| (1,1905) | 1:18:A:LEU:HD13 | 1:27:A:TYR:HD2 | 11       | 0.11          |
| (1,1905) | 1:18:A:LEU:HD21 | 1:27:A:TYR:HD1 | 11       | 0.11          |
| (1,1905) | 1:18:A:LEU:HD21 | 1:27:A:TYR:HD2 | 11       | 0.11          |
| (1,1905) | 1:18:A:LEU:HD22 | 1:27:A:TYR:HD1 | 11       | 0.11          |
| (1,1905) | 1:18:A:LEU:HD22 | 1:27:A:TYR:HD2 | 11       | 0.11          |
| (1,1905) | 1:18:A:LEU:HD23 | 1:27:A:TYR:HD1 | 11       | 0.11          |
| (1,1905) | 1:18:A:LEU:HD23 | 1:27:A:TYR:HD2 | 11       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD11 | 1:25:A:LEU:HG  | 15       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD12 | 1:25:A:LEU:HG  | 15       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD13 | 1:25:A:LEU:HG  | 15       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD21 | 1:25:A:LEU:HG  | 15       | 0.11          |

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| Key      | Atom-1          | Atom-2            | Model ID | Violation (Å) |
|----------|-----------------|-------------------|----------|---------------|
| (1,1898) | 1:18:A:LEU:HD22 | 1:25:A:LEU:HG     | 15       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD23 | 1:25:A:LEU:HG     | 15       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD11 | 1:25:A:LEU:HG     | 17       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD12 | 1:25:A:LEU:HG     | 17       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD13 | 1:25:A:LEU:HG     | 17       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD21 | 1:25:A:LEU:HG     | 17       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD22 | 1:25:A:LEU:HG     | 17       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD23 | 1:25:A:LEU:HG     | 17       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD11 | 1:25:A:LEU:HG     | 18       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD12 | 1:25:A:LEU:HG     | 18       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD13 | 1:25:A:LEU:HG     | 18       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD21 | 1:25:A:LEU:HG     | 18       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD22 | 1:25:A:LEU:HG     | 18       | 0.11          |
| (1,1898) | 1:18:A:LEU:HD23 | 1:25:A:LEU:HG     | 18       | 0.11          |
| (1,1888) | 1:18:A:LEU:H    | 1:25:A:LEU:HD11   | 11       | 0.11          |
| (1,1888) | 1:18:A:LEU:H    | 1:25:A:LEU:HD12   | 11       | 0.11          |
| (1,1888) | 1:18:A:LEU:H    | 1:25:A:LEU:HD13   | 11       | 0.11          |
| (1,1888) | 1:18:A:LEU:H    | 1:25:A:LEU:HD21   | 11       | 0.11          |
| (1,1888) | 1:18:A:LEU:H    | 1:25:A:LEU:HD22   | 11       | 0.11          |
| (1,1888) | 1:18:A:LEU:H    | 1:25:A:LEU:HD23   | 11       | 0.11          |
| (1,1888) | 1:18:A:LEU:H    | 1:25:A:LEU:HD11   | 19       | 0.11          |
| (1,1888) | 1:18:A:LEU:H    | 1:25:A:LEU:HD12   | 19       | 0.11          |
| (1,1888) | 1:18:A:LEU:H    | 1:25:A:LEU:HD13   | 19       | 0.11          |
| (1,1888) | 1:18:A:LEU:H    | 1:25:A:LEU:HD21   | 19       | 0.11          |
| (1,1888) | 1:18:A:LEU:H    | 1:25:A:LEU:HD22   | 19       | 0.11          |
| (1,1888) | 1:18:A:LEU:H    | 1:25:A:LEU:HD23   | 19       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG21 | 1        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG22 | 1        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG23 | 1        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG21 | 3        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG22 | 3        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG23 | 3        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG21 | 4        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG22 | 4        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG23 | 4        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG21 | 6        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG22 | 6        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG23 | 6        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG21 | 7        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG22 | 7        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG23 | 7        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1  | 1:1568:A:ILE:HG21 | 8        | 0.11          |

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| Key      | Atom-1         | Atom-2            | Model ID | Violation (Å) |
|----------|----------------|-------------------|----------|---------------|
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG22 | 8        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG23 | 8        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG21 | 9        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG22 | 9        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG23 | 9        | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG21 | 12       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG22 | 12       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG23 | 12       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG21 | 13       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG22 | 13       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG23 | 13       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG21 | 14       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG22 | 14       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG23 | 14       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG21 | 16       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG22 | 16       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG23 | 16       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG21 | 17       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG22 | 17       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG23 | 17       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG21 | 18       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG22 | 18       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG23 | 18       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG21 | 19       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG22 | 19       | 0.11          |
| (1,1782) | 1:42:A:TRP:HE1 | 1:1568:A:ILE:HG23 | 19       | 0.11          |
| (1,1494) | 1:27:A:TYR:HE1 | 1:34:A:ILE:HG21   | 9        | 0.11          |
| (1,1494) | 1:27:A:TYR:HE1 | 1:34:A:ILE:HG22   | 9        | 0.11          |
| (1,1494) | 1:27:A:TYR:HE1 | 1:34:A:ILE:HG23   | 9        | 0.11          |
| (1,1494) | 1:27:A:TYR:HE2 | 1:34:A:ILE:HG21   | 9        | 0.11          |
| (1,1494) | 1:27:A:TYR:HE2 | 1:34:A:ILE:HG22   | 9        | 0.11          |
| (1,1494) | 1:27:A:TYR:HE2 | 1:34:A:ILE:HG23   | 9        | 0.11          |
| (1,1441) | 1:25:A:LEU:HB2 | 1:1568:A:ILE:HD11 | 11       | 0.11          |
| (1,1441) | 1:25:A:LEU:HB2 | 1:1568:A:ILE:HD12 | 11       | 0.11          |
| (1,1441) | 1:25:A:LEU:HB2 | 1:1568:A:ILE:HD13 | 11       | 0.11          |
| (1,1441) | 1:25:A:LEU:HB2 | 1:1568:A:ILE:HD11 | 19       | 0.11          |
| (1,1441) | 1:25:A:LEU:HB2 | 1:1568:A:ILE:HD12 | 19       | 0.11          |
| (1,1441) | 1:25:A:LEU:HB2 | 1:1568:A:ILE:HD13 | 19       | 0.11          |
| (1,1409) | 1:11:A:ALA:HB1 | 1:12:A:LEU:HD11   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB1 | 1:12:A:LEU:HD12   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB1 | 1:12:A:LEU:HD13   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB1 | 1:12:A:LEU:HD21   | 8        | 0.11          |

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| Key      | Atom-1          | Atom-2            | Model ID | Violation (Å) |
|----------|-----------------|-------------------|----------|---------------|
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD22   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD23   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD11   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD12   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD13   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD21   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD22   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD23   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB3  | 1:12:A:LEU:HD11   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB3  | 1:12:A:LEU:HD12   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB3  | 1:12:A:LEU:HD13   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB3  | 1:12:A:LEU:HD21   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB3  | 1:12:A:LEU:HD22   | 8        | 0.11          |
| (1,1409) | 1:11:A:ALA:HB3  | 1:12:A:LEU:HD23   | 8        | 0.11          |
| (1,1363) | 1:26:A:GLN:HA   | 1:1568:A:ILE:HG21 | 8        | 0.11          |
| (1,1363) | 1:26:A:GLN:HA   | 1:1568:A:ILE:HG22 | 8        | 0.11          |
| (1,1363) | 1:26:A:GLN:HA   | 1:1568:A:ILE:HG23 | 8        | 0.11          |
| (1,1359) | 1:7:A:ILE:HG21  | 1:49:A:LEU:HA     | 5        | 0.11          |
| (1,1359) | 1:7:A:ILE:HG22  | 1:49:A:LEU:HA     | 5        | 0.11          |
| (1,1359) | 1:7:A:ILE:HG23  | 1:49:A:LEU:HA     | 5        | 0.11          |
| (1,1359) | 1:7:A:ILE:HG21  | 1:49:A:LEU:HA     | 6        | 0.11          |
| (1,1359) | 1:7:A:ILE:HG22  | 1:49:A:LEU:HA     | 6        | 0.11          |
| (1,1359) | 1:7:A:ILE:HG23  | 1:49:A:LEU:HA     | 6        | 0.11          |
| (1,1359) | 1:7:A:ILE:HG21  | 1:49:A:LEU:HA     | 9        | 0.11          |
| (1,1359) | 1:7:A:ILE:HG22  | 1:49:A:LEU:HA     | 9        | 0.11          |
| (1,1359) | 1:7:A:ILE:HG23  | 1:49:A:LEU:HA     | 9        | 0.11          |
| (1,1359) | 1:7:A:ILE:HG21  | 1:49:A:LEU:HA     | 14       | 0.11          |
| (1,1359) | 1:7:A:ILE:HG22  | 1:49:A:LEU:HA     | 14       | 0.11          |
| (1,1359) | 1:7:A:ILE:HG23  | 1:49:A:LEU:HA     | 14       | 0.11          |
| (1,1359) | 1:7:A:ILE:HG21  | 1:49:A:LEU:HA     | 16       | 0.11          |
| (1,1359) | 1:7:A:ILE:HG22  | 1:49:A:LEU:HA     | 16       | 0.11          |
| (1,1359) | 1:7:A:ILE:HG23  | 1:49:A:LEU:HA     | 16       | 0.11          |
| (1,1317) | 1:18:A:LEU:H    | 1:18:A:LEU:HD21   | 7        | 0.11          |
| (1,1317) | 1:18:A:LEU:H    | 1:18:A:LEU:HD22   | 7        | 0.11          |
| (1,1317) | 1:18:A:LEU:H    | 1:18:A:LEU:HD23   | 7        | 0.11          |
| (1,1310) | 1:20:A:VAL:HG11 | 1:24:A:ARG:H      | 13       | 0.11          |
| (1,1310) | 1:20:A:VAL:HG12 | 1:24:A:ARG:H      | 13       | 0.11          |
| (1,1310) | 1:20:A:VAL:HG13 | 1:24:A:ARG:H      | 13       | 0.11          |
| (1,1228) | 1:34:A:ILE:HD11 | 1:39:A:LEU:HD21   | 3        | 0.11          |
| (1,1228) | 1:34:A:ILE:HD11 | 1:39:A:LEU:HD22   | 3        | 0.11          |
| (1,1228) | 1:34:A:ILE:HD11 | 1:39:A:LEU:HD23   | 3        | 0.11          |
| (1,1228) | 1:34:A:ILE:HD12 | 1:39:A:LEU:HD21   | 3        | 0.11          |

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| Key      | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|----------|-------------------|------------------|----------|---------------|
| (1,1228) | 1:34:A:ILE:HD12   | 1:39:A:LEU:HD22  | 3        | 0.11          |
| (1,1228) | 1:34:A:ILE:HD12   | 1:39:A:LEU:HD23  | 3        | 0.11          |
| (1,1228) | 1:34:A:ILE:HD13   | 1:39:A:LEU:HD21  | 3        | 0.11          |
| (1,1228) | 1:34:A:ILE:HD13   | 1:39:A:LEU:HD22  | 3        | 0.11          |
| (1,1228) | 1:34:A:ILE:HD13   | 1:39:A:LEU:HD23  | 3        | 0.11          |
| (1,1212) | 1:2:A:ILE:HG12    | 1:7:A:ILE:HG21   | 2        | 0.11          |
| (1,1212) | 1:2:A:ILE:HG12    | 1:7:A:ILE:HG22   | 2        | 0.11          |
| (1,1212) | 1:2:A:ILE:HG12    | 1:7:A:ILE:HG23   | 2        | 0.11          |
| (1,1178) | 1:16:A:ILE:HD11   | 1:35:A:PRO:HG3   | 5        | 0.11          |
| (1,1178) | 1:16:A:ILE:HD12   | 1:35:A:PRO:HG3   | 5        | 0.11          |
| (1,1178) | 1:16:A:ILE:HD13   | 1:35:A:PRO:HG3   | 5        | 0.11          |
| (1,1153) | 1:1556:A:GLU:H    | 1:1556:A:GLU:HB3 | 2        | 0.11          |
| (1,853)  | 1:12:A:LEU:HA     | 1:16:A:ILE:HD11  | 3        | 0.11          |
| (1,853)  | 1:12:A:LEU:HA     | 1:16:A:ILE:HD12  | 3        | 0.11          |
| (1,853)  | 1:12:A:LEU:HA     | 1:16:A:ILE:HD13  | 3        | 0.11          |
| (1,90)   | 1:1545:A:LEU:H    | 1:1547:A:LYS:H   | 2        | 0.11          |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H   | 4        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H   | 4        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H   | 4        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H   | 4        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H   | 4        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H   | 4        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H   | 6        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H   | 6        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H   | 6        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H   | 6        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H   | 6        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H   | 6        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H   | 7        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H   | 7        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H   | 7        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H   | 7        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H   | 7        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H   | 7        | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H   | 11       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H   | 11       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H   | 11       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H   | 11       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H   | 11       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H   | 11       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H   | 15       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H   | 15       | 0.1           |

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| Key      | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|----------|-------------------|------------------|----------|---------------|
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H   | 15       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H   | 15       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H   | 15       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H   | 15       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD11 | 1:1566:A:GLY:H   | 19       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD12 | 1:1566:A:GLY:H   | 19       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD13 | 1:1566:A:GLY:H   | 19       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD21 | 1:1566:A:GLY:H   | 19       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD22 | 1:1566:A:GLY:H   | 19       | 0.1           |
| (1,2225) | 1:1564:A:LEU:HD23 | 1:1566:A:GLY:H   | 19       | 0.1           |
| (1,2223) | 1:1564:A:LEU:HD11 | 1:1565:A:ARG:H   | 14       | 0.1           |
| (1,2223) | 1:1564:A:LEU:HD12 | 1:1565:A:ARG:H   | 14       | 0.1           |
| (1,2223) | 1:1564:A:LEU:HD13 | 1:1565:A:ARG:H   | 14       | 0.1           |
| (1,2223) | 1:1564:A:LEU:HD21 | 1:1565:A:ARG:H   | 14       | 0.1           |
| (1,2223) | 1:1564:A:LEU:HD22 | 1:1565:A:ARG:H   | 14       | 0.1           |
| (1,2223) | 1:1564:A:LEU:HD23 | 1:1565:A:ARG:H   | 14       | 0.1           |
| (1,2182) | 1:1550:A:ARG:H    | 1:1550:A:ARG:HG2 | 17       | 0.1           |
| (1,2182) | 1:1550:A:ARG:H    | 1:1550:A:ARG:HG3 | 17       | 0.1           |
| (1,2136) | 1:63:A:LYS:HB2    | 1:64:A:GLY:HA2   | 19       | 0.1           |
| (1,2136) | 1:63:A:LYS:HB2    | 1:64:A:GLY:HA3   | 19       | 0.1           |
| (1,2136) | 1:63:A:LYS:HB3    | 1:64:A:GLY:HA2   | 19       | 0.1           |
| (1,2136) | 1:63:A:LYS:HB3    | 1:64:A:GLY:HA3   | 19       | 0.1           |
| (1,2099) | 1:54:A:ASN:HB3    | 1:55:A:GLN:HB2   | 2        | 0.1           |
| (1,2099) | 1:54:A:ASN:HB3    | 1:55:A:GLN:HB3   | 2        | 0.1           |
| (1,2056) | 1:47:A:GLN:HG2    | 1:50:A:ILE:HG21  | 16       | 0.1           |
| (1,2056) | 1:47:A:GLN:HG2    | 1:50:A:ILE:HG22  | 16       | 0.1           |
| (1,2056) | 1:47:A:GLN:HG2    | 1:50:A:ILE:HG23  | 16       | 0.1           |
| (1,2056) | 1:47:A:GLN:HG3    | 1:50:A:ILE:HG21  | 16       | 0.1           |
| (1,2056) | 1:47:A:GLN:HG3    | 1:50:A:ILE:HG22  | 16       | 0.1           |
| (1,2056) | 1:47:A:GLN:HG3    | 1:50:A:ILE:HG23  | 16       | 0.1           |
| (1,2033) | 1:42:A:TRP:HD1    | 1:49:A:LEU:HD11  | 1        | 0.1           |
| (1,2033) | 1:42:A:TRP:HD1    | 1:49:A:LEU:HD12  | 1        | 0.1           |
| (1,2033) | 1:42:A:TRP:HD1    | 1:49:A:LEU:HD13  | 1        | 0.1           |
| (1,2033) | 1:42:A:TRP:HD1    | 1:49:A:LEU:HD21  | 1        | 0.1           |
| (1,2033) | 1:42:A:TRP:HD1    | 1:49:A:LEU:HD22  | 1        | 0.1           |
| (1,2033) | 1:42:A:TRP:HD1    | 1:49:A:LEU:HD23  | 1        | 0.1           |
| (1,2033) | 1:42:A:TRP:HD1    | 1:49:A:LEU:HD11  | 12       | 0.1           |
| (1,2033) | 1:42:A:TRP:HD1    | 1:49:A:LEU:HD12  | 12       | 0.1           |
| (1,2033) | 1:42:A:TRP:HD1    | 1:49:A:LEU:HD13  | 12       | 0.1           |
| (1,2033) | 1:42:A:TRP:HD1    | 1:49:A:LEU:HD21  | 12       | 0.1           |
| (1,2033) | 1:42:A:TRP:HD1    | 1:49:A:LEU:HD22  | 12       | 0.1           |
| (1,2033) | 1:42:A:TRP:HD1    | 1:49:A:LEU:HD23  | 12       | 0.1           |

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| Key      | Atom-1          | Atom-2            | Model ID | Violation (Å) |
|----------|-----------------|-------------------|----------|---------------|
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD11 | 5        | 0.1           |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD12 | 5        | 0.1           |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD13 | 5        | 0.1           |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD21 | 5        | 0.1           |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD22 | 5        | 0.1           |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD23 | 5        | 0.1           |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD11 | 11       | 0.1           |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD12 | 11       | 0.1           |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD13 | 11       | 0.1           |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD21 | 11       | 0.1           |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD22 | 11       | 0.1           |
| (1,1996) | 1:32:A:ASP:HA   | 1:1564:A:LEU:HD23 | 11       | 0.1           |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD11   | 4        | 0.1           |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD12   | 4        | 0.1           |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD13   | 4        | 0.1           |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD21   | 4        | 0.1           |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD22   | 4        | 0.1           |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD23   | 4        | 0.1           |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD11   | 10       | 0.1           |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD12   | 10       | 0.1           |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD13   | 10       | 0.1           |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD21   | 10       | 0.1           |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD22   | 10       | 0.1           |
| (1,1974) | 1:26:A:GLN:H    | 1:53:A:LEU:HD23   | 10       | 0.1           |
| (1,1972) | 1:25:A:LEU:HD11 | 1:1568:A:ILE:HG12 | 11       | 0.1           |
| (1,1972) | 1:25:A:LEU:HD12 | 1:1568:A:ILE:HG12 | 11       | 0.1           |
| (1,1972) | 1:25:A:LEU:HD13 | 1:1568:A:ILE:HG12 | 11       | 0.1           |
| (1,1972) | 1:25:A:LEU:HD21 | 1:1568:A:ILE:HG12 | 11       | 0.1           |
| (1,1972) | 1:25:A:LEU:HD22 | 1:1568:A:ILE:HG12 | 11       | 0.1           |
| (1,1972) | 1:25:A:LEU:HD23 | 1:1568:A:ILE:HG12 | 11       | 0.1           |
| (1,1958) | 1:25:A:LEU:HD11 | 1:49:A:LEU:H      | 1        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD12 | 1:49:A:LEU:H      | 1        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD13 | 1:49:A:LEU:H      | 1        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD21 | 1:49:A:LEU:H      | 1        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD22 | 1:49:A:LEU:H      | 1        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD23 | 1:49:A:LEU:H      | 1        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD11 | 1:49:A:LEU:H      | 6        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD12 | 1:49:A:LEU:H      | 6        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD13 | 1:49:A:LEU:H      | 6        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD21 | 1:49:A:LEU:H      | 6        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD22 | 1:49:A:LEU:H      | 6        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD23 | 1:49:A:LEU:H      | 6        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1958) | 1:25:A:LEU:HD11 | 1:49:A:LEU:H    | 7        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD12 | 1:49:A:LEU:H    | 7        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD13 | 1:49:A:LEU:H    | 7        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD21 | 1:49:A:LEU:H    | 7        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD22 | 1:49:A:LEU:H    | 7        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD23 | 1:49:A:LEU:H    | 7        | 0.1           |
| (1,1958) | 1:25:A:LEU:HD11 | 1:49:A:LEU:H    | 13       | 0.1           |
| (1,1958) | 1:25:A:LEU:HD12 | 1:49:A:LEU:H    | 13       | 0.1           |
| (1,1958) | 1:25:A:LEU:HD13 | 1:49:A:LEU:H    | 13       | 0.1           |
| (1,1958) | 1:25:A:LEU:HD21 | 1:49:A:LEU:H    | 13       | 0.1           |
| (1,1958) | 1:25:A:LEU:HD22 | 1:49:A:LEU:H    | 13       | 0.1           |
| (1,1958) | 1:25:A:LEU:HD23 | 1:49:A:LEU:H    | 13       | 0.1           |
| (1,1958) | 1:25:A:LEU:HD11 | 1:49:A:LEU:H    | 20       | 0.1           |
| (1,1958) | 1:25:A:LEU:HD12 | 1:49:A:LEU:H    | 20       | 0.1           |
| (1,1958) | 1:25:A:LEU:HD13 | 1:49:A:LEU:H    | 20       | 0.1           |
| (1,1958) | 1:25:A:LEU:HD21 | 1:49:A:LEU:H    | 20       | 0.1           |
| (1,1958) | 1:25:A:LEU:HD22 | 1:49:A:LEU:H    | 20       | 0.1           |
| (1,1958) | 1:25:A:LEU:HD23 | 1:49:A:LEU:H    | 20       | 0.1           |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD11 | 16       | 0.1           |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD12 | 16       | 0.1           |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD13 | 16       | 0.1           |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD21 | 16       | 0.1           |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD22 | 16       | 0.1           |
| (1,1946) | 1:24:A:ARG:H    | 1:25:A:LEU:HD23 | 16       | 0.1           |
| (1,1943) | 1:21:A:VAL:HG11 | 1:26:A:GLN:H    | 17       | 0.1           |
| (1,1943) | 1:21:A:VAL:HG12 | 1:26:A:GLN:H    | 17       | 0.1           |
| (1,1943) | 1:21:A:VAL:HG13 | 1:26:A:GLN:H    | 17       | 0.1           |
| (1,1943) | 1:21:A:VAL:HG21 | 1:26:A:GLN:H    | 17       | 0.1           |
| (1,1943) | 1:21:A:VAL:HG22 | 1:26:A:GLN:H    | 17       | 0.1           |
| (1,1943) | 1:21:A:VAL:HG23 | 1:26:A:GLN:H    | 17       | 0.1           |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD11 | 8        | 0.1           |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD12 | 8        | 0.1           |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD13 | 8        | 0.1           |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD21 | 8        | 0.1           |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD22 | 8        | 0.1           |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD23 | 8        | 0.1           |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD11 | 10       | 0.1           |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD12 | 10       | 0.1           |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD13 | 10       | 0.1           |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD21 | 10       | 0.1           |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD22 | 10       | 0.1           |
| (1,1934) | 1:21:A:VAL:H    | 1:25:A:LEU:HD23 | 10       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD11 | 3        | 0.1           |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD12 | 3        | 0.1           |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD13 | 3        | 0.1           |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD21 | 3        | 0.1           |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD22 | 3        | 0.1           |
| (1,1923) | 1:19:A:PHE:HE1  | 1:56:A:LEU:HD23 | 3        | 0.1           |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD11 | 3        | 0.1           |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD12 | 3        | 0.1           |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD13 | 3        | 0.1           |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD21 | 3        | 0.1           |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD22 | 3        | 0.1           |
| (1,1923) | 1:19:A:PHE:HE2  | 1:56:A:LEU:HD23 | 3        | 0.1           |
| (1,1906) | 1:18:A:LEU:HD11 | 1:42:A:TRP:H    | 15       | 0.1           |
| (1,1906) | 1:18:A:LEU:HD12 | 1:42:A:TRP:H    | 15       | 0.1           |
| (1,1906) | 1:18:A:LEU:HD13 | 1:42:A:TRP:H    | 15       | 0.1           |
| (1,1906) | 1:18:A:LEU:HD21 | 1:42:A:TRP:H    | 15       | 0.1           |
| (1,1906) | 1:18:A:LEU:HD22 | 1:42:A:TRP:H    | 15       | 0.1           |
| (1,1906) | 1:18:A:LEU:HD23 | 1:42:A:TRP:H    | 15       | 0.1           |
| (1,1898) | 1:18:A:LEU:HD11 | 1:25:A:LEU:HG   | 3        | 0.1           |
| (1,1898) | 1:18:A:LEU:HD12 | 1:25:A:LEU:HG   | 3        | 0.1           |
| (1,1898) | 1:18:A:LEU:HD13 | 1:25:A:LEU:HG   | 3        | 0.1           |
| (1,1898) | 1:18:A:LEU:HD21 | 1:25:A:LEU:HG   | 3        | 0.1           |
| (1,1898) | 1:18:A:LEU:HD22 | 1:25:A:LEU:HG   | 3        | 0.1           |
| (1,1898) | 1:18:A:LEU:HD23 | 1:25:A:LEU:HG   | 3        | 0.1           |
| (1,1898) | 1:18:A:LEU:HD11 | 1:25:A:LEU:HG   | 14       | 0.1           |
| (1,1898) | 1:18:A:LEU:HD12 | 1:25:A:LEU:HG   | 14       | 0.1           |
| (1,1898) | 1:18:A:LEU:HD13 | 1:25:A:LEU:HG   | 14       | 0.1           |
| (1,1898) | 1:18:A:LEU:HD21 | 1:25:A:LEU:HG   | 14       | 0.1           |
| (1,1898) | 1:18:A:LEU:HD22 | 1:25:A:LEU:HG   | 14       | 0.1           |
| (1,1898) | 1:18:A:LEU:HD23 | 1:25:A:LEU:HG   | 14       | 0.1           |
| (1,1886) | 1:17:A:THR:HG21 | 1:18:A:LEU:HD11 | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG21 | 1:18:A:LEU:HD12 | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG21 | 1:18:A:LEU:HD13 | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG21 | 1:18:A:LEU:HD21 | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG21 | 1:18:A:LEU:HD22 | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG21 | 1:18:A:LEU:HD23 | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG22 | 1:18:A:LEU:HD11 | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG22 | 1:18:A:LEU:HD12 | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG22 | 1:18:A:LEU:HD13 | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG22 | 1:18:A:LEU:HD21 | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG22 | 1:18:A:LEU:HD22 | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG22 | 1:18:A:LEU:HD23 | 3        | 0.1           |

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| Key      | Atom-1          | Atom-2            | Model ID | Violation (Å) |
|----------|-----------------|-------------------|----------|---------------|
| (1,1886) | 1:17:A:THR:HG23 | 1:18:A:LEU:HD11   | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG23 | 1:18:A:LEU:HD12   | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG23 | 1:18:A:LEU:HD13   | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG23 | 1:18:A:LEU:HD21   | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG23 | 1:18:A:LEU:HD22   | 3        | 0.1           |
| (1,1886) | 1:17:A:THR:HG23 | 1:18:A:LEU:HD23   | 3        | 0.1           |
| (1,1719) | 1:21:A:VAL:H    | 1:50:A:ILE:HD11   | 15       | 0.1           |
| (1,1719) | 1:21:A:VAL:H    | 1:50:A:ILE:HD12   | 15       | 0.1           |
| (1,1719) | 1:21:A:VAL:H    | 1:50:A:ILE:HD13   | 15       | 0.1           |
| (1,1657) | 1:14:A:GLN:HA   | 1:38:A:LEU:HD21   | 5        | 0.1           |
| (1,1657) | 1:14:A:GLN:HA   | 1:38:A:LEU:HD22   | 5        | 0.1           |
| (1,1657) | 1:14:A:GLN:HA   | 1:38:A:LEU:HD23   | 5        | 0.1           |
| (1,1657) | 1:14:A:GLN:HA   | 1:38:A:LEU:HD21   | 10       | 0.1           |
| (1,1657) | 1:14:A:GLN:HA   | 1:38:A:LEU:HD22   | 10       | 0.1           |
| (1,1657) | 1:14:A:GLN:HA   | 1:38:A:LEU:HD23   | 10       | 0.1           |
| (1,1562) | 1:16:A:ILE:HB   | 1:18:A:LEU:HD11   | 15       | 0.1           |
| (1,1562) | 1:16:A:ILE:HB   | 1:18:A:LEU:HD12   | 15       | 0.1           |
| (1,1562) | 1:16:A:ILE:HB   | 1:18:A:LEU:HD13   | 15       | 0.1           |
| (1,1562) | 1:16:A:ILE:HB   | 1:18:A:LEU:HD11   | 17       | 0.1           |
| (1,1562) | 1:16:A:ILE:HB   | 1:18:A:LEU:HD12   | 17       | 0.1           |
| (1,1562) | 1:16:A:ILE:HB   | 1:18:A:LEU:HD13   | 17       | 0.1           |
| (1,1554) | 1:16:A:ILE:HG21 | 1:27:A:TYR:HE1    | 7        | 0.1           |
| (1,1554) | 1:16:A:ILE:HG21 | 1:27:A:TYR:HE2    | 7        | 0.1           |
| (1,1554) | 1:16:A:ILE:HG22 | 1:27:A:TYR:HE1    | 7        | 0.1           |
| (1,1554) | 1:16:A:ILE:HG22 | 1:27:A:TYR:HE2    | 7        | 0.1           |
| (1,1554) | 1:16:A:ILE:HG23 | 1:27:A:TYR:HE1    | 7        | 0.1           |
| (1,1554) | 1:16:A:ILE:HG23 | 1:27:A:TYR:HE2    | 7        | 0.1           |
| (1,1441) | 1:25:A:LEU:HB2  | 1:1568:A:ILE:HD11 | 8        | 0.1           |
| (1,1441) | 1:25:A:LEU:HB2  | 1:1568:A:ILE:HD12 | 8        | 0.1           |
| (1,1441) | 1:25:A:LEU:HB2  | 1:1568:A:ILE:HD13 | 8        | 0.1           |
| (1,1430) | 1:25:A:LEU:HB2  | 1:50:A:ILE:HG21   | 8        | 0.1           |
| (1,1430) | 1:25:A:LEU:HB2  | 1:50:A:ILE:HG22   | 8        | 0.1           |
| (1,1430) | 1:25:A:LEU:HB2  | 1:50:A:ILE:HG23   | 8        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD11   | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD12   | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD13   | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD21   | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD22   | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB1  | 1:12:A:LEU:HD23   | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD11   | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD12   | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB2  | 1:12:A:LEU:HD13   | 4        | 0.1           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1409) | 1:11:A:ALA:HB2 | 1:12:A:LEU:HD21 | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB2 | 1:12:A:LEU:HD22 | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB2 | 1:12:A:LEU:HD23 | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB3 | 1:12:A:LEU:HD11 | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB3 | 1:12:A:LEU:HD12 | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB3 | 1:12:A:LEU:HD13 | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB3 | 1:12:A:LEU:HD21 | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB3 | 1:12:A:LEU:HD22 | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB3 | 1:12:A:LEU:HD23 | 4        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB1 | 1:12:A:LEU:HD11 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB1 | 1:12:A:LEU:HD12 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB1 | 1:12:A:LEU:HD13 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB1 | 1:12:A:LEU:HD21 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB1 | 1:12:A:LEU:HD22 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB1 | 1:12:A:LEU:HD23 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB2 | 1:12:A:LEU:HD11 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB2 | 1:12:A:LEU:HD12 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB2 | 1:12:A:LEU:HD13 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB2 | 1:12:A:LEU:HD21 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB2 | 1:12:A:LEU:HD22 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB2 | 1:12:A:LEU:HD23 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB3 | 1:12:A:LEU:HD11 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB3 | 1:12:A:LEU:HD12 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB3 | 1:12:A:LEU:HD13 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB3 | 1:12:A:LEU:HD21 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB3 | 1:12:A:LEU:HD22 | 9        | 0.1           |
| (1,1409) | 1:11:A:ALA:HB3 | 1:12:A:LEU:HD23 | 9        | 0.1           |
| (1,1359) | 1:7:A:ILE:HG21 | 1:49:A:LEU:HA   | 3        | 0.1           |
| (1,1359) | 1:7:A:ILE:HG22 | 1:49:A:LEU:HA   | 3        | 0.1           |
| (1,1359) | 1:7:A:ILE:HG23 | 1:49:A:LEU:HA   | 3        | 0.1           |
| (1,1359) | 1:7:A:ILE:HG21 | 1:49:A:LEU:HA   | 7        | 0.1           |
| (1,1359) | 1:7:A:ILE:HG22 | 1:49:A:LEU:HA   | 7        | 0.1           |
| (1,1359) | 1:7:A:ILE:HG23 | 1:49:A:LEU:HA   | 7        | 0.1           |
| (1,1359) | 1:7:A:ILE:HG21 | 1:49:A:LEU:HA   | 10       | 0.1           |
| (1,1359) | 1:7:A:ILE:HG22 | 1:49:A:LEU:HA   | 10       | 0.1           |
| (1,1359) | 1:7:A:ILE:HG23 | 1:49:A:LEU:HA   | 10       | 0.1           |
| (1,1359) | 1:7:A:ILE:HG21 | 1:49:A:LEU:HA   | 15       | 0.1           |
| (1,1359) | 1:7:A:ILE:HG22 | 1:49:A:LEU:HA   | 15       | 0.1           |
| (1,1359) | 1:7:A:ILE:HG23 | 1:49:A:LEU:HA   | 15       | 0.1           |
| (1,1359) | 1:7:A:ILE:HG21 | 1:49:A:LEU:HA   | 17       | 0.1           |
| (1,1359) | 1:7:A:ILE:HG22 | 1:49:A:LEU:HA   | 17       | 0.1           |
| (1,1359) | 1:7:A:ILE:HG23 | 1:49:A:LEU:HA   | 17       | 0.1           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1359) | 1:7:A:ILE:HG21   | 1:49:A:LEU:HA   | 20       | 0.1           |
| (1,1359) | 1:7:A:ILE:HG22   | 1:49:A:LEU:HA   | 20       | 0.1           |
| (1,1359) | 1:7:A:ILE:HG23   | 1:49:A:LEU:HA   | 20       | 0.1           |
| (1,1291) | 1:16:A:ILE:HG21  | 1:38:A:LEU:HD11 | 10       | 0.1           |
| (1,1291) | 1:16:A:ILE:HG21  | 1:38:A:LEU:HD12 | 10       | 0.1           |
| (1,1291) | 1:16:A:ILE:HG21  | 1:38:A:LEU:HD13 | 10       | 0.1           |
| (1,1291) | 1:16:A:ILE:HG22  | 1:38:A:LEU:HD11 | 10       | 0.1           |
| (1,1291) | 1:16:A:ILE:HG22  | 1:38:A:LEU:HD12 | 10       | 0.1           |
| (1,1291) | 1:16:A:ILE:HG22  | 1:38:A:LEU:HD13 | 10       | 0.1           |
| (1,1291) | 1:16:A:ILE:HG23  | 1:38:A:LEU:HD11 | 10       | 0.1           |
| (1,1291) | 1:16:A:ILE:HG23  | 1:38:A:LEU:HD12 | 10       | 0.1           |
| (1,1291) | 1:16:A:ILE:HG23  | 1:38:A:LEU:HD13 | 10       | 0.1           |
| (1,1231) | 1:63:A:LYS:HG3   | 1:64:A:GLY:HA2  | 17       | 0.1           |
| (1,1231) | 1:63:A:LYS:HG3   | 1:64:A:GLY:HA3  | 17       | 0.1           |
| (1,1228) | 1:34:A:ILE:HD11  | 1:39:A:LEU:HD21 | 15       | 0.1           |
| (1,1228) | 1:34:A:ILE:HD11  | 1:39:A:LEU:HD22 | 15       | 0.1           |
| (1,1228) | 1:34:A:ILE:HD11  | 1:39:A:LEU:HD23 | 15       | 0.1           |
| (1,1228) | 1:34:A:ILE:HD12  | 1:39:A:LEU:HD21 | 15       | 0.1           |
| (1,1228) | 1:34:A:ILE:HD12  | 1:39:A:LEU:HD22 | 15       | 0.1           |
| (1,1228) | 1:34:A:ILE:HD12  | 1:39:A:LEU:HD23 | 15       | 0.1           |
| (1,1228) | 1:34:A:ILE:HD13  | 1:39:A:LEU:HD21 | 15       | 0.1           |
| (1,1228) | 1:34:A:ILE:HD13  | 1:39:A:LEU:HD22 | 15       | 0.1           |
| (1,1228) | 1:34:A:ILE:HD13  | 1:39:A:LEU:HD23 | 15       | 0.1           |
| (1,1178) | 1:16:A:ILE:HD11  | 1:35:A:PRO:HG3  | 10       | 0.1           |
| (1,1178) | 1:16:A:ILE:HD12  | 1:35:A:PRO:HG3  | 10       | 0.1           |
| (1,1178) | 1:16:A:ILE:HD13  | 1:35:A:PRO:HG3  | 10       | 0.1           |
| (1,1166) | 1:63:A:LYS:HD2   | 1:64:A:GLY:HA2  | 11       | 0.1           |
| (1,1166) | 1:63:A:LYS:HD2   | 1:64:A:GLY:HA3  | 11       | 0.1           |
| (1,1166) | 1:63:A:LYS:HD3   | 1:64:A:GLY:HA2  | 11       | 0.1           |
| (1,1166) | 1:63:A:LYS:HD3   | 1:64:A:GLY:HA3  | 11       | 0.1           |
| (1,1126) | 1:1548:A:GLU:HG2 | 1:1549:A:LYS:HA | 6        | 0.1           |
| (1,1126) | 1:1548:A:GLU:HG3 | 1:1549:A:LYS:HA | 6        | 0.1           |
| (1,1126) | 1:1548:A:GLU:HG2 | 1:1549:A:LYS:HA | 11       | 0.1           |
| (1,1126) | 1:1548:A:GLU:HG3 | 1:1549:A:LYS:HA | 11       | 0.1           |
| (1,1087) | 1:36:A:THR:HG21  | 1:40:A:ASN:HB2  | 8        | 0.1           |
| (1,1087) | 1:36:A:THR:HG22  | 1:40:A:ASN:HB2  | 8        | 0.1           |
| (1,1087) | 1:36:A:THR:HG23  | 1:40:A:ASN:HB2  | 8        | 0.1           |
| (1,617)  | 1:16:A:ILE:H     | 1:34:A:ILE:HD11 | 2        | 0.1           |
| (1,617)  | 1:16:A:ILE:H     | 1:34:A:ILE:HD12 | 2        | 0.1           |
| (1,617)  | 1:16:A:ILE:H     | 1:34:A:ILE:HD13 | 2        | 0.1           |
| (1,387)  | 1:1555:A:ALA:HB1 | 1:1556:A:GLU:H  | 19       | 0.1           |
| (1,387)  | 1:1555:A:ALA:HB2 | 1:1556:A:GLU:H  | 19       | 0.1           |

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| Key     | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|---------|------------------|----------------|----------|---------------|
| (1,387) | 1:1555:A:ALA:HB3 | 1:1556:A:GLU:H | 19       | 0.1           |
| (1,172) | 1:12:A:LEU:HD11  | 1:13:A:GLU:H   | 20       | 0.1           |
| (1,172) | 1:12:A:LEU:HD12  | 1:13:A:GLU:H   | 20       | 0.1           |
| (1,172) | 1:12:A:LEU:HD13  | 1:13:A:GLU:H   | 20       | 0.1           |
| (1,172) | 1:12:A:LEU:HD21  | 1:13:A:GLU:H   | 20       | 0.1           |
| (1,172) | 1:12:A:LEU:HD22  | 1:13:A:GLU:H   | 20       | 0.1           |
| (1,172) | 1:12:A:LEU:HD23  | 1:13:A:GLU:H   | 20       | 0.1           |
| (1,63)  | 1:25:A:LEU:HD21  | 1:26:A:GLN:H   | 19       | 0.1           |
| (1,63)  | 1:25:A:LEU:HD22  | 1:26:A:GLN:H   | 19       | 0.1           |
| (1,63)  | 1:25:A:LEU:HD23  | 1:26:A:GLN:H   | 19       | 0.1           |

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

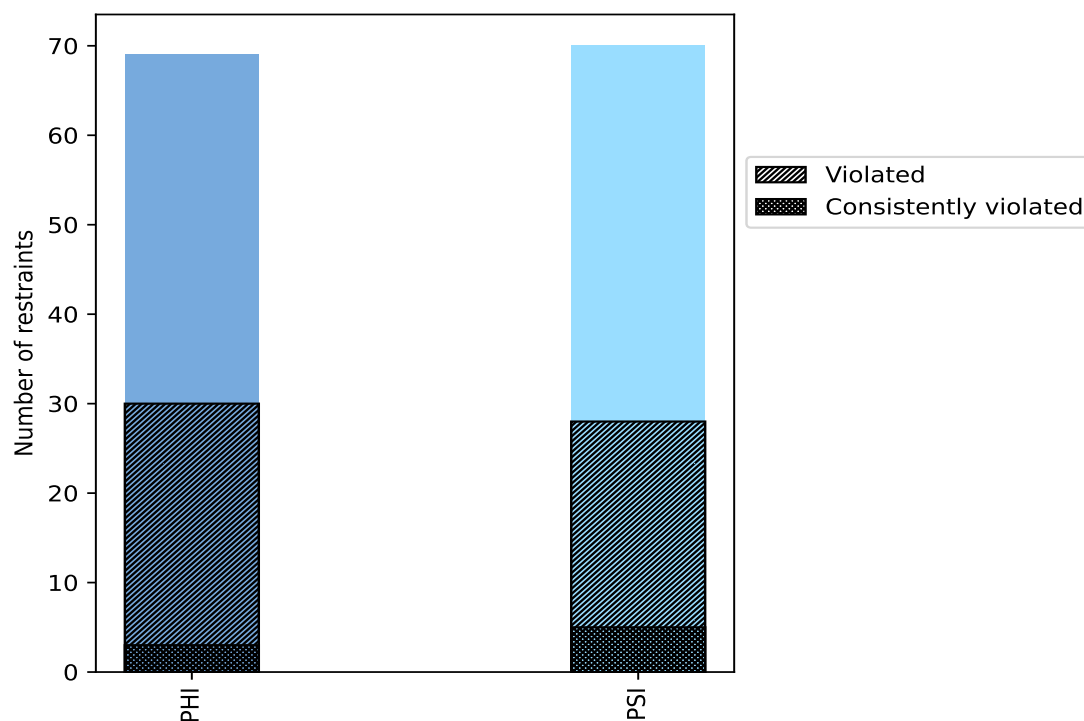
### 10.1 Summary of dihedral-angle violations [i](#)

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> |
| PHI        | 69    | 49.6           | 30                    | 43.5           | 21.6           | 3                                  | 4.3            | 2.2            |
| PSI        | 70    | 50.4           | 28                    | 40.0           | 20.1           | 5                                  | 7.1            | 3.6            |
| Total      | 139   | 100.0          | 58                    | 41.7           | 41.7           | 8                                  | 5.8            | 5.8            |

<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](#)



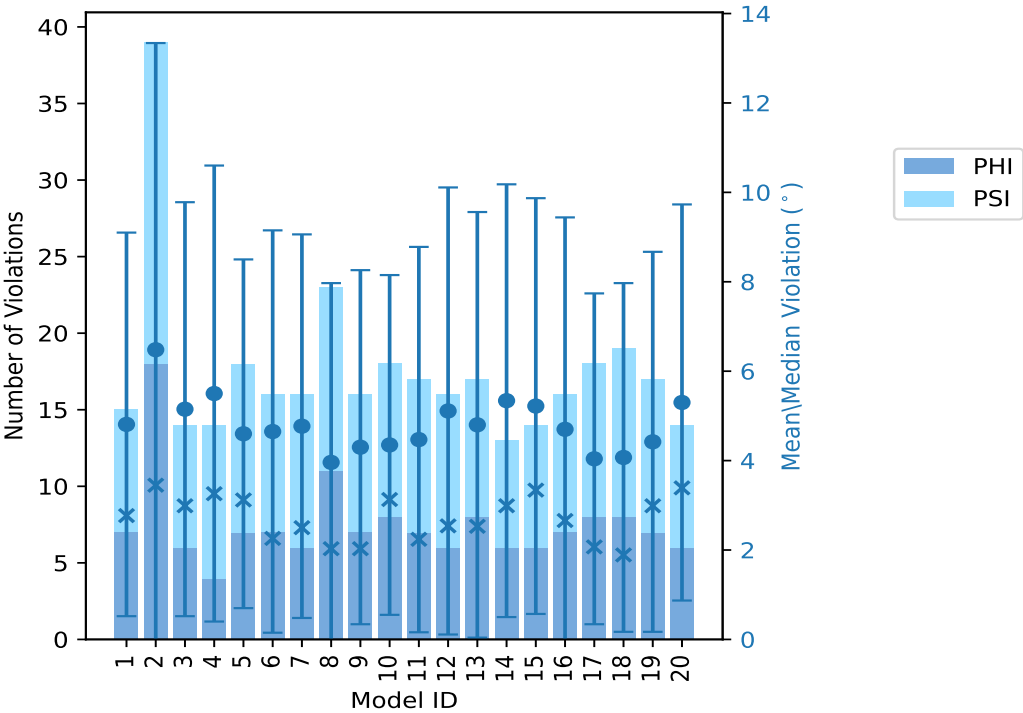
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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 (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 7                    | 8   | 15    | 4.81     | 15.51   | 4.29   | 2.77       |
| 2        | 18                   | 21  | 39    | 6.48     | 34.55   | 6.86   | 3.45       |
| 3        | 6                    | 8   | 14    | 5.15     | 16.01   | 4.63   | 2.99       |
| 4        | 4                    | 10  | 14    | 5.5      | 16.95   | 5.1    | 3.26       |
| 5        | 7                    | 11  | 18    | 4.6      | 14.61   | 3.9    | 3.12       |
| 6        | 7                    | 9   | 16    | 4.65     | 15.86   | 4.5    | 2.26       |
| 7        | 6                    | 10  | 16    | 4.77     | 14.68   | 4.29   | 2.5        |
| 8        | 11                   | 12  | 23    | 3.96     | 15.17   | 4.01   | 2.03       |
| 9        | 7                    | 9   | 16    | 4.3      | 13.2    | 3.96   | 2.03       |
| 10       | 8                    | 10  | 18    | 4.35     | 13.59   | 3.8    | 3.13       |
| 11       | 7                    | 10  | 17    | 4.47     | 14.59   | 4.31   | 2.24       |
| 12       | 6                    | 10  | 16    | 5.11     | 18.14   | 5.0    | 2.54       |
| 13       | 8                    | 9   | 17    | 4.8      | 15.54   | 4.76   | 2.53       |
| 14       | 6                    | 7   | 13    | 5.34     | 16.28   | 4.84   | 2.99       |
| 15       | 6                    | 8   | 14    | 5.22     | 16.65   | 4.65   | 3.34       |
| 16       | 7                    | 9   | 16    | 4.7      | 16.18   | 4.74   | 2.66       |
| 17       | 8                    | 10  | 18    | 4.04     | 13.78   | 3.7    | 2.07       |
| 18       | 8                    | 11  | 19    | 4.07     | 14.91   | 3.9    | 1.89       |
| 19       | 7                    | 10  | 17    | 4.42     | 14.81   | 4.25   | 2.99       |
| 20       | 6                    | 8   | 14    | 5.3      | 15.25   | 4.43   | 3.39       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %    |
| 13                            | 10  | 23    | 1                        | 5.0  |
| 6                             | 2   | 8     | 2                        | 10.0 |
| 5                             | 2   | 7     | 3                        | 15.0 |
| 0                             | 3   | 3     | 4                        | 20.0 |
| 0                             | 1   | 1     | 5                        | 25.0 |
| 0                             | 1   | 1     | 6                        | 30.0 |
| 0                             | 0   | 0     | 7                        | 35.0 |
| 0                             | 1   | 1     | 8                        | 40.0 |
| 0                             | 0   | 0     | 9                        | 45.0 |
| 0                             | 0   | 0     | 10                       | 50.0 |
| 0                             | 0   | 0     | 11                       | 55.0 |

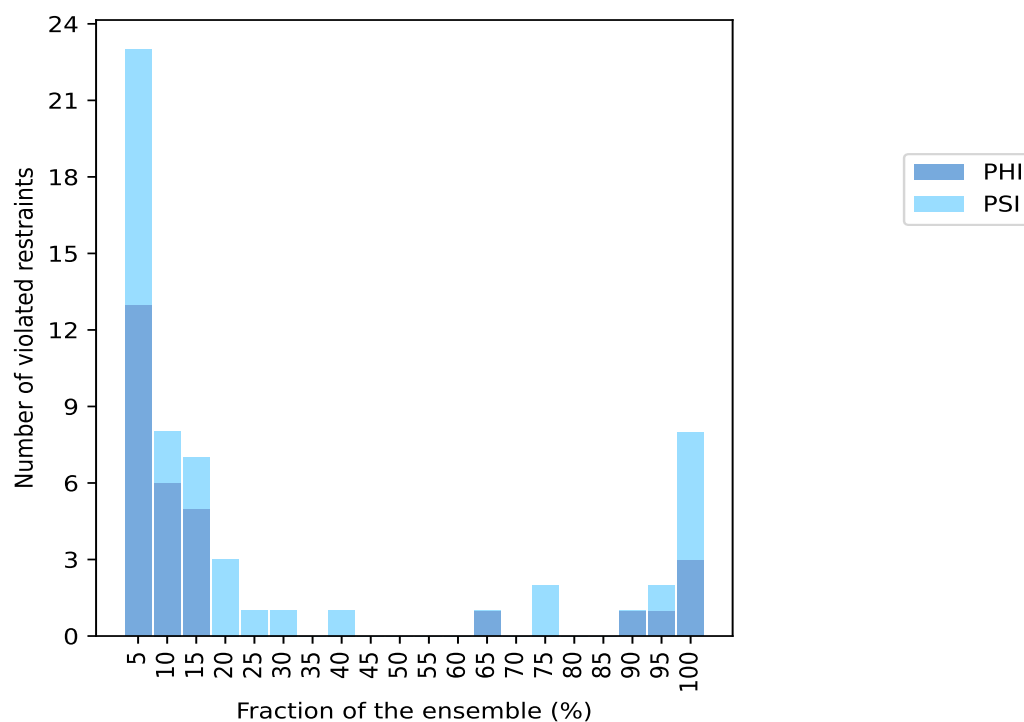
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0     | 12                       | 60.0  |
| 1                             | 0   | 1     | 13                       | 65.0  |
| 0                             | 0   | 0     | 14                       | 70.0  |
| 0                             | 2   | 2     | 15                       | 75.0  |
| 0                             | 0   | 0     | 16                       | 80.0  |
| 0                             | 0   | 0     | 17                       | 85.0  |
| 1                             | 0   | 1     | 18                       | 90.0  |
| 1                             | 1   | 2     | 19                       | 95.0  |
| 3                             | 5   | 8     | 20                       | 100.0 |

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

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

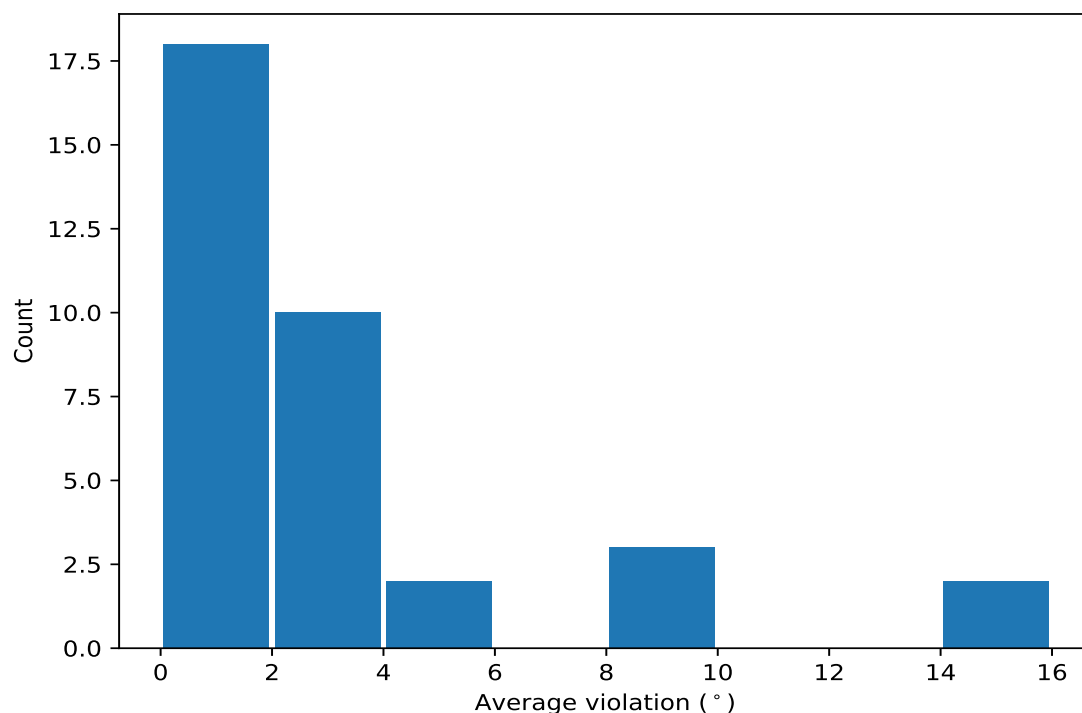


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

| Key     | Atom-1         | Atom-2          | Atom-3         | Atom-4         | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Med  |
|---------|----------------|-----------------|----------------|----------------|---------------------|-------|-----------------|------|
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 1:32:A:ASP:N   | 20                  | 15.53 | 1.6             | 15.3 |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA  | 1:32:A:ASP:C   | 20                  | 14.39 | 2.14            | 14.3 |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA  | 1:31:A:ARG:C   | 20                  | 8.56  | 1.54            | 8.6  |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C   | 1:31:A:ARG:N   | 20                  | 8.13  | 1.71            | 7.8  |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 1:33:A:SER:N   | 20                  | 5.63  | 1.22            | 5.6  |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 20                  | 5.01  | 1.45            | 4.6  |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA   | 1:19:A:PHE:C   | 1:20:A:VAL:N   | 20                  | 2.93  | 1.16            | 2.8  |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C   | 1:37:A:GLU:N   | 20                  | 1.85  | 0.51            | 1.7  |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N    | 1:30:A:SER:CA  | 1:30:A:SER:C   | 19                  | 3.55  | 0.73            | 3.4  |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA   | 1:37:A:GLU:C   | 1:38:A:LEU:N   | 19                  | 2.7   | 1.27            | 2.5  |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA  | 1:38:A:LEU:C   | 18                  | 2.52  | 1.65            | 2.1  |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C   | 1:25:A:LEU:N   | 15                  | 1.73  | 0.65            | 1.4  |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C   | 1:43:A:LYS:N   | 15                  | 1.71  | 1.05            | 1.3  |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N     | 1:3:A:ASP:CA   | 1:3:A:ASP:C    | 13                  | 1.6   | 0.51            | 1.4  |
| (1,28)  | 1:16:A:ILE:N   | 1:16:A:ILE:CA   | 1:16:A:ILE:C   | 1:17:A:THR:N   | 8                   | 1.44  | 0.43            | 1.3  |
| (1,123) | 1:1550:A:ARG:N | 1:1550:A:ARG:CA | 1:1550:A:ARG:C | 1:1551:A:LYS:N | 6                   | 1.36  | 0.18            | 1.3  |
| (1,131) | 1:1554:A:GLN:N | 1:1554:A:GLN:CA | 1:1554:A:GLN:C | 1:1555:A:ALA:N | 5                   | 8.19  | 13.18           | 1.6  |
| (1,133) | 1:1563:A:TYR:N | 1:1563:A:TYR:CA | 1:1563:A:TYR:C | 1:1564:A:LEU:N | 4                   | 2.98  | 2.48            | 1.8  |
| (1,30)  | 1:17:A:THR:N   | 1:17:A:THR:CA   | 1:17:A:THR:C   | 1:18:A:LEU:N   | 4                   | 2.77  | 1.27            | 2.8  |
| (1,94)  | 1:51:A:ASP:N   | 1:51:A:ASP:CA   | 1:51:A:ASP:C   | 1:52:A:PHE:N   | 4                   | 1.35  | 0.19            | 1.2  |

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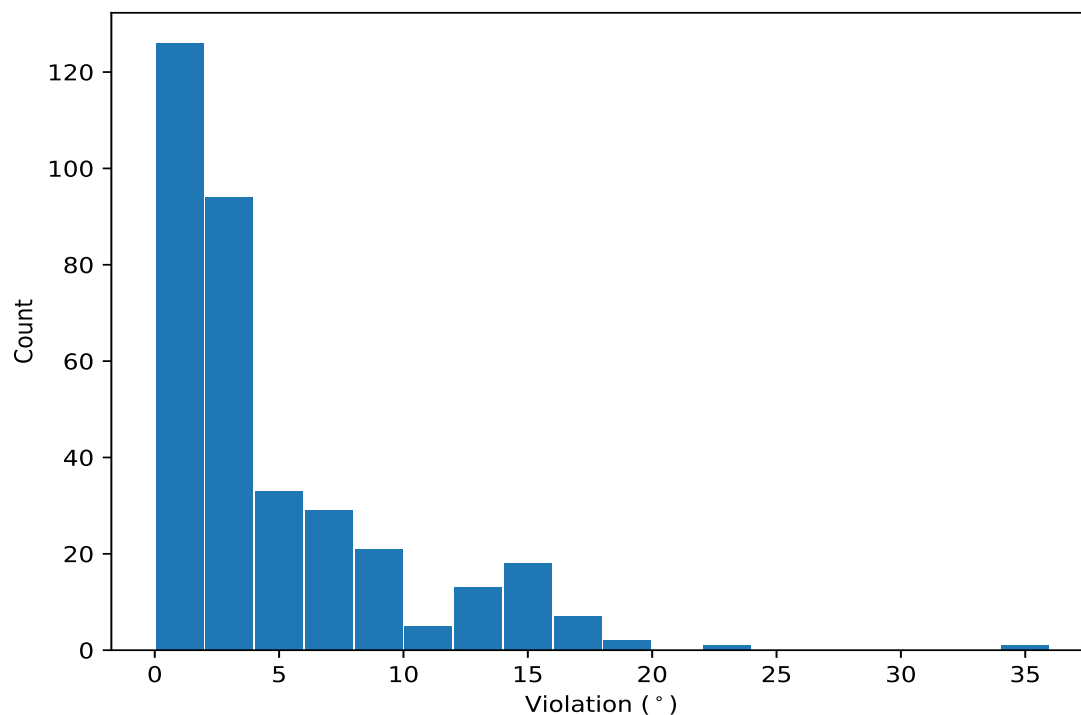
| Key     | Atom-1         | Atom-2          | Atom-3          | Atom-4         | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Med |
|---------|----------------|-----------------|-----------------|----------------|---------------------|------|-----------------|-----|
| (1,49)  | 1:26:A:GLN:C   | 1:27:A:TYR:N    | 1:27:A:TYR:CA   | 1:27:A:TYR:C   | 3                   | 2.25 | 0.64            | 2.0 |
| (1,137) | 1:1565:A:ARG:N | 1:1565:A:ARG:CA | 1:1565:A:ARG:C  | 1:1566:A:GLY:N | 3                   | 1.59 | 0.26            | 1.5 |
| (1,93)  | 1:50:A:ILE:C   | 1:51:A:ASP:N    | 1:51:A:ASP:CA   | 1:51:A:ASP:C   | 3                   | 1.48 | 0.52            | 1.2 |
| (1,116) | 1:1546:A:LEU:C | 1:1547:A:LYS:N  | 1:1547:A:LYS:CA | 1:1547:A:LYS:C | 3                   | 1.45 | 0.22            | 1.4 |
| (1,119) | 1:1548:A:GLU:N | 1:1548:A:GLU:CA | 1:1548:A:GLU:C  | 1:1549:A:LYS:N | 3                   | 1.33 | 0.11            | 1.3 |
| (1,134) | 1:1563:A:TYR:C | 1:1564:A:LEU:N  | 1:1564:A:LEU:CA | 1:1564:A:LEU:C | 3                   | 1.22 | 0.12            | 1.3 |
| (1,27)  | 1:15:A:GLY:C   | 1:16:A:ILE:N    | 1:16:A:ILE:CA   | 1:16:A:ILE:C   | 3                   | 1.2  | 0.26            | 1.0 |
| (1,118) | 1:1547:A:LYS:C | 1:1548:A:GLU:N  | 1:1548:A:GLU:CA | 1:1548:A:GLU:C | 2                   | 2.3  | 1.04            | 2.3 |
| (1,65)  | 1:36:A:THR:C   | 1:37:A:GLU:N    | 1:37:A:GLU:CA   | 1:37:A:GLU:C   | 2                   | 2.1  | 0.97            | 2.1 |
| (1,90)  | 1:49:A:LEU:N   | 1:49:A:LEU:CA   | 1:49:A:LEU:C    | 1:50:A:ILE:N   | 2                   | 2.08 | 0.15            | 2.0 |
| (1,109) | 1:58:A:SER:C   | 1:59:A:GLU:N    | 1:59:A:GLU:CA   | 1:59:A:GLU:C   | 2                   | 1.5  | 0.13            | 1.5 |
| (1,95)  | 1:51:A:ASP:C   | 1:52:A:PHE:N    | 1:52:A:PHE:CA   | 1:52:A:PHE:C   | 2                   | 1.42 | 0.1             | 1.4 |
| (1,111) | 1:59:A:GLU:C   | 1:60:A:GLU:N    | 1:60:A:GLU:CA   | 1:60:A:GLU:C   | 2                   | 1.38 | 0.24            | 1.3 |
| (1,61)  | 1:33:A:SER:C   | 1:34:A:ILE:N    | 1:34:A:ILE:CA   | 1:34:A:ILE:C   | 2                   | 1.17 | 0.05            | 1.1 |
| (1,46)  | 1:25:A:LEU:N   | 1:25:A:LEU:CA   | 1:25:A:LEU:C    | 1:26:A:GLN:N   | 2                   | 1.14 | 0.12            | 1.1 |

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

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

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

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





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

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

| Key     | Atom-1         | Atom-2          | Atom-3          | Atom-4         | Model ID | Violation (°) |
|---------|----------------|-----------------|-----------------|----------------|----------|---------------|
| (1,131) | 1:1554:A:GLN:N | 1:1554:A:GLN:CA | 1:1554:A:GLN:C  | 1:1555:A:ALA:N | 2        | 34.55         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 2        | 22.07         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 2        | 19.99         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 12       | 18.14         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 4        | 16.95         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 15       | 16.65         |
| (1,124) | 1:1550:A:ARG:C | 1:1551:A:LYS:N  | 1:1551:A:LYS:CA | 1:1551:A:LYS:C | 2        | 16.37         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 14       | 16.28         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 16       | 16.18         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 16       | 16.15         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 3        | 16.01         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 6        | 15.86         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 13       | 15.54         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 13       | 15.53         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 1        | 15.51         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 20       | 15.25         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 8        | 15.17         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 12       | 15.0          |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 6        | 14.92         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 8        | 14.91         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 18       | 14.91         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 4        | 14.85         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 19       | 14.81         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 19       | 14.77         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 7        | 14.68         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 5        | 14.61         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 11       | 14.59         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 5        | 14.42         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 15       | 14.34         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 3        | 13.87         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 17       | 13.78         |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 2        | 13.78         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 1        | 13.76         |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 2        | 13.67         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 11       | 13.62         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 10       | 13.59         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 7        | 13.43         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 20       | 13.31         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 14       | 13.3          |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 9        | 13.2          |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 10       | 13.08         |
| (1,58)  | 1:31:A:ARG:N   | 1:31:A:ARG:CA   | 1:31:A:ARG:C    | 1:32:A:ASP:N   | 9        | 12.91         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 18       | 11.53         |
| (1,59)  | 1:31:A:ARG:C   | 1:32:A:ASP:N    | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 17       | 10.93         |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA   | 1:20:A:VAL:C   | 2        | 10.73         |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 13       | 10.2          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 11       | 10.02         |

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| Key     | Atom-1         | Atom-2          | Atom-3          | Atom-4         | Model ID | Violation (°) |
|---------|----------------|-----------------|-----------------|----------------|----------|---------------|
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 4        | 9.88          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 14       | 9.65          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 4        | 9.48          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 12       | 9.47          |
| (1,125) | 1:1551:A:LYS:N | 1:1551:A:LYS:CA | 1:1551:A:LYS:C  | 1:1552:A:HIS:N | 2        | 9.28          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 18       | 9.02          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 10       | 8.89          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 17       | 8.89          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 3        | 8.74          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 2        | 8.72          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 13       | 8.72          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 20       | 8.71          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 7        | 8.71          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 14       | 8.71          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 20       | 8.66          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 9        | 8.55          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 7        | 8.39          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 11       | 8.28          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 8        | 8.16          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 9        | 8.12          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 18       | 8.07          |
| (1,114) | 1:1545:A:LEU:C | 1:1546:A:LEU:N  | 1:1546:A:LEU:CA | 1:1546:A:LEU:C | 2        | 7.82          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 17       | 7.7           |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 8        | 7.69          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA   | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 2        | 7.59          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 19       | 7.51          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C    | 1:33:A:SER:N   | 13       | 7.5           |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 12       | 7.48          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 19       | 7.31          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 5        | 7.3           |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 16       | 7.29          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA   | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 2        | 7.29          |
| (1,133) | 1:1563:A:TYR:N | 1:1563:A:TYR:CA | 1:1563:A:TYR:C  | 1:1564:A:LEU:N | 2        | 7.24          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C    | 1:33:A:SER:N   | 8        | 7.23          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 3        | 7.23          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C    | 1:33:A:SER:N   | 6        | 7.08          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 16       | 7.01          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 1        | 6.99          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 15       | 6.99          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 6        | 6.83          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C    | 1:33:A:SER:N   | 3        | 6.71          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C    | 1:33:A:SER:N   | 7        | 6.68          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 5        | 6.65          |
| (1,57)  | 1:30:A:SER:C   | 1:31:A:ARG:N    | 1:31:A:ARG:CA   | 1:31:A:ARG:C   | 15       | 6.57          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C    | 1:33:A:SER:N   | 12       | 6.46          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C    | 1:33:A:SER:N   | 15       | 6.46          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 10       | 6.44          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C    | 1:33:A:SER:N   | 1        | 6.37          |
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C    | 1:31:A:ARG:N   | 6        | 6.21          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N    | 1:30:A:SER:CA   | 1:30:A:SER:C   | 2        | 6.13          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA   | 1:20:A:VAL:C   | 20       | 5.92          |

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| Key     | Atom-1         | Atom-2          | Atom-3         | Atom-4         | Model ID | Violation (°) |
|---------|----------------|-----------------|----------------|----------------|----------|---------------|
| (1,56)  | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C   | 1:31:A:ARG:N   | 1        | 5.85          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 1:33:A:SER:N   | 5        | 5.78          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 12       | 5.76          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 1:33:A:SER:N   | 11       | 5.68          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 1:33:A:SER:N   | 4        | 5.55          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 1:33:A:SER:N   | 20       | 5.49          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C   | 1:43:A:LYS:N   | 2        | 5.47          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 1:33:A:SER:N   | 17       | 5.44          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 10       | 5.42          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 4        | 5.3           |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 18       | 5.29          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 1:33:A:SER:N   | 16       | 5.24          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 7        | 5.2           |
| (1,127) | 1:1552:A:HIS:N | 1:1552:A:HIS:CA | 1:1552:A:HIS:C | 1:1553:A:PHE:N | 2        | 5.17          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 1:33:A:SER:N   | 10       | 5.09          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 15       | 4.95          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 1        | 4.87          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 8        | 4.77          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 1:33:A:SER:N   | 18       | 4.67          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 5        | 4.61          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 14       | 4.52          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 1:33:A:SER:N   | 14       | 4.5           |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 19       | 4.47          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 1:33:A:SER:N   | 19       | 4.45          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 16       | 4.31          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 9        | 4.21          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 6        | 4.2           |
| (1,30)  | 1:17:A:THR:N   | 1:17:A:THR:CA   | 1:17:A:THR:C   | 1:18:A:LEU:N   | 2        | 4.14          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N    | 1:30:A:SER:CA  | 1:30:A:SER:C   | 7        | 4.1           |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 13       | 4.09          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N    | 1:30:A:SER:CA  | 1:30:A:SER:C   | 10       | 4.06          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 17       | 4.02          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N    | 1:30:A:SER:CA  | 1:30:A:SER:C   | 8        | 3.95          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 11       | 3.93          |
| (1,30)  | 1:17:A:THR:N   | 1:17:A:THR:CA   | 1:17:A:THR:C   | 1:18:A:LEU:N   | 5        | 3.9           |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N    | 1:30:A:SER:CA  | 1:30:A:SER:C   | 1        | 3.89          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N    | 1:30:A:SER:CA  | 1:30:A:SER:C   | 6        | 3.71          |
| (1,121) | 1:1549:A:LYS:N | 1:1549:A:LYS:CA | 1:1549:A:LYS:C | 1:1550:A:ARG:N | 2        | 3.69          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N    | 1:30:A:SER:CA  | 1:30:A:SER:C   | 5        | 3.65          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA   | 1:32:A:ASP:C   | 1:33:A:SER:N   | 9        | 3.62          |
| (1,35)  | 1:19:A:PHE:C   | 1:20:A:VAL:N    | 1:20:A:VAL:CA  | 1:20:A:VAL:C   | 3        | 3.56          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA   | 1:19:A:PHE:C   | 1:20:A:VAL:N   | 18       | 3.56          |
| (1,26)  | 1:15:A:GLY:N   | 1:15:A:GLY:CA   | 1:15:A:GLY:C   | 1:16:A:ILE:N   | 2        | 3.56          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C   | 1:25:A:LEU:N   | 8        | 3.53          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA  | 1:38:A:LEU:C   | 10       | 3.51          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N    | 1:30:A:SER:CA  | 1:30:A:SER:C   | 15       | 3.5           |
| (1,19)  | 1:11:A:ALA:C   | 1:12:A:LEU:N    | 1:12:A:LEU:CA  | 1:12:A:LEU:C   | 2        | 3.45          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA  | 1:38:A:LEU:C   | 19       | 3.43          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA   | 1:19:A:PHE:C   | 1:20:A:VAL:N   | 12       | 3.42          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N    | 1:30:A:SER:CA  | 1:30:A:SER:C   | 4        | 3.4           |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N    | 1:30:A:SER:CA  | 1:30:A:SER:C   | 17       | 3.4           |

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| Key     | Atom-1         | Atom-2         | Atom-3          | Atom-4         | Model ID | Violation (°) |
|---------|----------------|----------------|-----------------|----------------|----------|---------------|
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C   | 20       | 3.4           |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA  | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 20       | 3.38          |
| (1,39)  | 1:21:A:VAL:C   | 1:22:A:ASN:N   | 1:22:A:ASN:CA   | 1:22:A:ASN:C   | 2        | 3.36          |
| (1,118) | 1:1547:A:LYS:C | 1:1548:A:GLU:N | 1:1548:A:GLU:CA | 1:1548:A:GLU:C | 2        | 3.33          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C   | 11       | 3.32          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA  | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 17       | 3.27          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C   | 13       | 3.25          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA  | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 10       | 3.21          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA  | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 15       | 3.19          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA  | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 8        | 3.19          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA  | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 5        | 3.13          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA  | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 4        | 3.12          |
| (1,49)  | 1:26:A:GLN:C   | 1:27:A:TYR:N   | 1:27:A:TYR:CA   | 1:27:A:TYR:C   | 5        | 3.11          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA  | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 19       | 3.1           |
| (1,65)  | 1:36:A:THR:C   | 1:37:A:GLU:N   | 1:37:A:GLU:CA   | 1:37:A:GLU:C   | 2        | 3.07          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C   | 16       | 3.07          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA  | 1:36:A:THR:C    | 1:37:A:GLU:N   | 10       | 3.05          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA  | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 3        | 3.04          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C   | 18       | 3.01          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N   | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 5        | 3.0           |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C   | 9        | 3.0           |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C   | 19       | 2.99          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA  | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 14       | 2.99          |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N    | 1:3:A:ASP:CA    | 1:3:A:ASP:C    | 18       | 2.99          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N   | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 3        | 2.93          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA  | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 16       | 2.93          |
| (1,73)  | 1:40:A:ASN:C   | 1:41:A:LYS:N   | 1:41:A:LYS:CA   | 1:41:A:LYS:C   | 2        | 2.83          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C   | 12       | 2.8           |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA  | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 15       | 2.79          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA  | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 1        | 2.77          |
| (1,55)  | 1:29:A:THR:C   | 1:30:A:SER:N   | 1:30:A:SER:CA   | 1:30:A:SER:C   | 3        | 2.76          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA  | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 19       | 2.75          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA  | 1:36:A:THR:C    | 1:37:A:GLU:N   | 2        | 2.75          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA  | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 8        | 2.71          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA  | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 13       | 2.71          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA  | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 7        | 2.65          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA  | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 20       | 2.63          |
| (1,60)  | 1:32:A:ASP:N   | 1:32:A:ASP:CA  | 1:32:A:ASP:C    | 1:33:A:SER:N   | 2        | 2.61          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N   | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 8        | 2.6           |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA  | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 11       | 2.6           |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA  | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 10       | 2.54          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA  | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 13       | 2.53          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA  | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 1        | 2.47          |
| (1,28)  | 1:16:A:ILE:N   | 1:16:A:ILE:CA  | 1:16:A:ILE:C    | 1:17:A:THR:N   | 5        | 2.39          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N   | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 16       | 2.38          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA  | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 6        | 2.38          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA  | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 7        | 2.36          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA  | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 5        | 2.35          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA  | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 12       | 2.29          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA  | 1:36:A:THR:C    | 1:37:A:GLU:N   | 20       | 2.28          |
| (1,97)  | 1:52:A:PHE:C   | 1:53:A:LEU:N   | 1:53:A:LEU:CA   | 1:53:A:LEU:C   | 2        | 2.25          |

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| Key     | Atom-1         | Atom-2          | Atom-3          | Atom-4         | Model ID | Violation (°) |
|---------|----------------|-----------------|-----------------|----------------|----------|---------------|
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 1        | 2.25          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA   | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 11       | 2.24          |
| (1,90)  | 1:49:A:LEU:N   | 1:49:A:LEU:CA   | 1:49:A:LEU:C    | 1:50:A:ILE:N   | 19       | 2.23          |
| (1,93)  | 1:50:A:ILE:C   | 1:51:A:ASP:N    | 1:51:A:ASP:CA   | 1:51:A:ASP:C   | 2        | 2.21          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 15       | 2.21          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 1        | 2.18          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 5        | 2.18          |
| (1,96)  | 1:52:A:PHE:N   | 1:52:A:PHE:CA   | 1:52:A:PHE:C    | 1:53:A:LEU:N   | 2        | 2.16          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 13       | 2.16          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 16       | 2.15          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 2        | 2.15          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 17       | 2.14          |
| (1,99)  | 1:53:A:LEU:C   | 1:54:A:ASN:N    | 1:54:A:ASN:CA   | 1:54:A:ASN:C   | 2        | 2.13          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA   | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 6        | 2.13          |
| (1,131) | 1:1554:A:GLN:N | 1:1554:A:GLN:CA | 1:1554:A:GLN:C  | 1:1555:A:ALA:N | 12       | 2.11          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 12       | 2.11          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 14       | 2.11          |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N     | 1:3:A:ASP:CA    | 1:3:A:ASP:C    | 6        | 2.09          |
| (1,49)  | 1:26:A:GLN:C   | 1:27:A:TYR:N    | 1:27:A:TYR:CA   | 1:27:A:TYR:C   | 2        | 2.08          |
| (1,133) | 1:1563:A:TYR:N | 1:1563:A:TYR:CA | 1:1563:A:TYR:C  | 1:1564:A:LEU:N | 9        | 2.05          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 7        | 2.05          |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N     | 1:3:A:ASP:CA    | 1:3:A:ASP:C    | 8        | 2.03          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA   | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 9        | 2.01          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 17       | 2.0           |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA   | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 9        | 1.99          |
| (1,70)  | 1:39:A:LEU:N   | 1:39:A:LEU:CA   | 1:39:A:LEU:C    | 1:40:A:ASN:N   | 2        | 1.98          |
| (1,137) | 1:1565:A:ARG:N | 1:1565:A:ARG:CA | 1:1565:A:ARG:C  | 1:1566:A:GLY:N | 12       | 1.93          |
| (1,90)  | 1:49:A:LEU:N   | 1:49:A:LEU:CA   | 1:49:A:LEU:C    | 1:50:A:ILE:N   | 11       | 1.93          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 16       | 1.93          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 4        | 1.91          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA   | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 18       | 1.89          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 13       | 1.83          |
| (1,30)  | 1:17:A:THR:N   | 1:17:A:THR:CA   | 1:17:A:THR:C    | 1:18:A:LEU:N   | 8        | 1.8           |
| (1,16)  | 1:10:A:GLU:N   | 1:10:A:GLU:CA   | 1:10:A:GLU:C    | 1:11:A:ALA:N   | 2        | 1.79          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 6        | 1.77          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 6        | 1.77          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 19       | 1.76          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 7        | 1.75          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA   | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 20       | 1.75          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 17       | 1.75          |
| (1,116) | 1:1546:A:LEU:C | 1:1547:A:LYS:N  | 1:1547:A:LYS:CA | 1:1547:A:LYS:C | 8        | 1.74          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 9        | 1.74          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 13       | 1.74          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 3        | 1.72          |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N     | 1:3:A:ASP:CA    | 1:3:A:ASP:C    | 10       | 1.71          |
| (1,28)  | 1:16:A:ILE:N   | 1:16:A:ILE:CA   | 1:16:A:ILE:C    | 1:17:A:THR:N   | 17       | 1.7           |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 11       | 1.69          |
| (1,40)  | 1:22:A:ASN:N   | 1:22:A:ASN:CA   | 1:22:A:ASN:C    | 1:23:A:ASN:N   | 2        | 1.68          |
| (1,94)  | 1:51:A:ASP:N   | 1:51:A:ASP:CA   | 1:51:A:ASP:C    | 1:52:A:PHE:N   | 17       | 1.67          |
| (1,131) | 1:1554:A:GLN:N | 1:1554:A:GLN:CA | 1:1554:A:GLN:C  | 1:1555:A:ALA:N | 14       | 1.66          |
| (1,123) | 1:1550:A:ARG:N | 1:1550:A:ARG:CA | 1:1550:A:ARG:C  | 1:1551:A:LYS:N | 16       | 1.66          |

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| Key     | Atom-1         | Atom-2          | Atom-3          | Atom-4         | Model ID | Violation (°) |
|---------|----------------|-----------------|-----------------|----------------|----------|---------------|
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 18       | 1.66          |
| (1,131) | 1:1554:A:GLN:N | 1:1554:A:GLN:CA | 1:1554:A:GLN:C  | 1:1555:A:ALA:N | 11       | 1.63          |
| (1,109) | 1:58:A:SER:C   | 1:59:A:GLU:N    | 1:59:A:GLU:CA   | 1:59:A:GLU:C   | 11       | 1.63          |
| (1,111) | 1:59:A:GLU:C   | 1:60:A:GLU:N    | 1:60:A:GLU:CA   | 1:60:A:GLU:C   | 14       | 1.62          |
| (1,74)  | 1:41:A:LYS:N   | 1:41:A:LYS:CA   | 1:41:A:LYS:C    | 1:42:A:TRP:N   | 2        | 1.59          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 18       | 1.59          |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N     | 1:3:A:ASP:CA    | 1:3:A:ASP:C    | 5        | 1.59          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 9        | 1.58          |
| (1,43)  | 1:23:A:ASN:C   | 1:24:A:ARG:N    | 1:24:A:ARG:CA   | 1:24:A:ARG:C   | 2        | 1.58          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA   | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 3        | 1.58          |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N     | 1:3:A:ASP:CA    | 1:3:A:ASP:C    | 9        | 1.58          |
| (1,49)  | 1:26:A:GLN:C   | 1:27:A:TYR:N    | 1:27:A:TYR:CA   | 1:27:A:TYR:C   | 18       | 1.57          |
| (1,27)  | 1:15:A:GLY:C   | 1:16:A:ILE:N    | 1:16:A:ILE:CA   | 1:16:A:ILE:C   | 16       | 1.57          |
| (1,137) | 1:1565:A:ARG:N | 1:1565:A:ARG:CA | 1:1565:A:ARG:C  | 1:1566:A:GLY:N | 8        | 1.55          |
| (1,133) | 1:1563:A:TYR:N | 1:1563:A:TYR:CA | 1:1563:A:TYR:C  | 1:1564:A:LEU:N | 4        | 1.55          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 9        | 1.55          |
| (1,28)  | 1:16:A:ILE:N   | 1:16:A:ILE:CA   | 1:16:A:ILE:C    | 1:17:A:THR:N   | 10       | 1.54          |
| (1,23)  | 1:13:A:GLU:C   | 1:14:A:GLN:N    | 1:14:A:GLN:CA   | 1:14:A:GLN:C   | 1        | 1.54          |
| (1,95)  | 1:51:A:ASP:C   | 1:52:A:PHE:N    | 1:52:A:PHE:CA   | 1:52:A:PHE:C   | 8        | 1.52          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA   | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 14       | 1.52          |
| (1,28)  | 1:16:A:ILE:N   | 1:16:A:ILE:CA   | 1:16:A:ILE:C    | 1:17:A:THR:N   | 12       | 1.51          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 5        | 1.5           |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 14       | 1.49          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 6        | 1.49          |
| (1,119) | 1:1548:A:GLU:N | 1:1548:A:GLU:CA | 1:1548:A:GLU:C  | 1:1549:A:LYS:N | 7        | 1.46          |
| (1,123) | 1:1550:A:ARG:N | 1:1550:A:ARG:CA | 1:1550:A:ARG:C  | 1:1551:A:LYS:N | 3        | 1.45          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 15       | 1.45          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 6        | 1.44          |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N     | 1:3:A:ASP:CA    | 1:3:A:ASP:C    | 3        | 1.44          |
| (1,123) | 1:1550:A:ARG:N | 1:1550:A:ARG:CA | 1:1550:A:ARG:C  | 1:1551:A:LYS:N | 5        | 1.42          |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N     | 1:3:A:ASP:CA    | 1:3:A:ASP:C    | 11       | 1.42          |
| (1,116) | 1:1546:A:LEU:C | 1:1547:A:LYS:N  | 1:1547:A:LYS:CA | 1:1547:A:LYS:C | 6        | 1.4           |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 1        | 1.4           |
| (1,25)  | 1:14:A:GLN:C   | 1:15:A:GLY:N    | 1:15:A:GLY:CA   | 1:15:A:GLY:C   | 2        | 1.38          |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N     | 1:3:A:ASP:CA    | 1:3:A:ASP:C    | 15       | 1.37          |
| (1,109) | 1:58:A:SER:C   | 1:59:A:GLU:N    | 1:59:A:GLU:CA   | 1:59:A:GLU:C   | 10       | 1.36          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 10       | 1.36          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 7        | 1.36          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 9        | 1.35          |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N     | 1:3:A:ASP:CA    | 1:3:A:ASP:C    | 13       | 1.35          |
| (1,123) | 1:1550:A:ARG:N | 1:1550:A:ARG:CA | 1:1550:A:ARG:C  | 1:1551:A:LYS:N | 8        | 1.34          |
| (1,119) | 1:1548:A:GLU:N | 1:1548:A:GLU:CA | 1:1548:A:GLU:C  | 1:1549:A:LYS:N | 17       | 1.33          |
| (1,95)  | 1:51:A:ASP:C   | 1:52:A:PHE:N    | 1:52:A:PHE:CA   | 1:52:A:PHE:C   | 17       | 1.32          |
| (1,134) | 1:1563:A:TYR:C | 1:1564:A:LEU:N  | 1:1564:A:LEU:CA | 1:1564:A:LEU:C | 9        | 1.31          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 8        | 1.31          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 15       | 1.31          |
| (1,66)  | 1:37:A:GLU:N   | 1:37:A:GLU:CA   | 1:37:A:GLU:C    | 1:38:A:LEU:N   | 4        | 1.31          |
| (1,137) | 1:1565:A:ARG:N | 1:1565:A:ARG:CA | 1:1565:A:ARG:C  | 1:1566:A:GLY:N | 18       | 1.3           |
| (1,134) | 1:1563:A:TYR:C | 1:1564:A:LEU:N  | 1:1564:A:LEU:CA | 1:1564:A:LEU:C | 18       | 1.3           |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 18       | 1.3           |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 4        | 1.3           |

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| Key     | Atom-1         | Atom-2          | Atom-3          | Atom-4         | Model ID | Violation (°) |
|---------|----------------|-----------------|-----------------|----------------|----------|---------------|
| (1,94)  | 1:51:A:ASP:N   | 1:51:A:ASP:CA   | 1:51:A:ASP:C    | 1:52:A:PHE:N   | 18       | 1.29          |
| (1,118) | 1:1547:A:LYS:C | 1:1548:A:GLU:N  | 1:1548:A:GLU:CA | 1:1548:A:GLU:C | 8        | 1.26          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 18       | 1.26          |
| (1,46)  | 1:25:A:LEU:N   | 1:25:A:LEU:CA   | 1:25:A:LEU:C    | 1:26:A:GLN:N   | 19       | 1.26          |
| (1,30)  | 1:17:A:THR:N   | 1:17:A:THR:CA   | 1:17:A:THR:C    | 1:18:A:LEU:N   | 15       | 1.25          |
| (1,94)  | 1:51:A:ASP:N   | 1:51:A:ASP:CA   | 1:51:A:ASP:C    | 1:52:A:PHE:N   | 7        | 1.23          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 13       | 1.23          |
| (1,51)  | 1:27:A:TYR:C   | 1:28:A:GLU:N    | 1:28:A:GLU:CA   | 1:28:A:GLU:C   | 8        | 1.23          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 10       | 1.23          |
| (1,61)  | 1:33:A:SER:C   | 1:34:A:ILE:N    | 1:34:A:ILE:CA   | 1:34:A:ILE:C   | 8        | 1.22          |
| (1,34)  | 1:19:A:PHE:N   | 1:19:A:PHE:CA   | 1:19:A:PHE:C    | 1:20:A:VAL:N   | 17       | 1.22          |
| (1,116) | 1:1546:A:LEU:C | 1:1547:A:LYS:N  | 1:1547:A:LYS:CA | 1:1547:A:LYS:C | 20       | 1.21          |
| (1,93)  | 1:50:A:ILE:C   | 1:51:A:ASP:N    | 1:51:A:ASP:CA   | 1:51:A:ASP:C   | 13       | 1.21          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 7        | 1.21          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 12       | 1.21          |
| (1,123) | 1:1550:A:ARG:N | 1:1550:A:ARG:CA | 1:1550:A:ARG:C  | 1:1551:A:LYS:N | 4        | 1.2           |
| (1,119) | 1:1548:A:GLU:N | 1:1548:A:GLU:CA | 1:1548:A:GLU:C  | 1:1549:A:LYS:N | 16       | 1.2           |
| (1,94)  | 1:51:A:ASP:N   | 1:51:A:ASP:CA   | 1:51:A:ASP:C    | 1:52:A:PHE:N   | 4        | 1.2           |
| (1,28)  | 1:16:A:ILE:N   | 1:16:A:ILE:CA   | 1:16:A:ILE:C    | 1:17:A:THR:N   | 20       | 1.2           |
| (1,92)  | 1:50:A:ILE:N   | 1:50:A:ILE:CA   | 1:50:A:ILE:C    | 1:51:A:ASP:N   | 2        | 1.19          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 19       | 1.19          |
| (1,67)  | 1:37:A:GLU:C   | 1:38:A:LEU:N    | 1:38:A:LEU:CA   | 1:38:A:LEU:C   | 11       | 1.18          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 5        | 1.18          |
| (1,111) | 1:59:A:GLU:C   | 1:60:A:GLU:N    | 1:60:A:GLU:CA   | 1:60:A:GLU:C   | 1        | 1.15          |
| (1,53)  | 1:28:A:GLU:C   | 1:29:A:THR:N    | 1:29:A:THR:CA   | 1:29:A:THR:C   | 17       | 1.14          |
| (1,65)  | 1:36:A:THR:C   | 1:37:A:GLU:N    | 1:37:A:GLU:CA   | 1:37:A:GLU:C   | 10       | 1.13          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 11       | 1.13          |
| (1,61)  | 1:33:A:SER:C   | 1:34:A:ILE:N    | 1:34:A:ILE:CA   | 1:34:A:ILE:C   | 7        | 1.12          |
| (1,103) | 1:55:A:GLN:C   | 1:56:A:LEU:N    | 1:56:A:LEU:CA   | 1:56:A:LEU:C   | 14       | 1.1           |
| (1,28)  | 1:16:A:ILE:N   | 1:16:A:ILE:CA   | 1:16:A:ILE:C    | 1:17:A:THR:N   | 6        | 1.1           |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N     | 1:3:A:ASP:CA    | 1:3:A:ASP:C    | 12       | 1.1           |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N     | 1:3:A:ASP:CA    | 1:3:A:ASP:C    | 17       | 1.1           |
| (1,133) | 1:1563:A:TYR:N | 1:1563:A:TYR:CA | 1:1563:A:TYR:C  | 1:1564:A:LEU:N | 18       | 1.09          |
| (1,123) | 1:1550:A:ARG:N | 1:1550:A:ARG:CA | 1:1550:A:ARG:C  | 1:1551:A:LYS:N | 1        | 1.09          |
| (1,44)  | 1:24:A:ARG:N   | 1:24:A:ARG:CA   | 1:24:A:ARG:C    | 1:25:A:LEU:N   | 19       | 1.09          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 8        | 1.06          |
| (1,1)   | 1:2:A:ILE:C    | 1:3:A:ASP:N     | 1:3:A:ASP:CA    | 1:3:A:ASP:C    | 19       | 1.06          |
| (1,134) | 1:1563:A:TYR:C | 1:1564:A:LEU:N  | 1:1564:A:LEU:CA | 1:1564:A:LEU:C | 16       | 1.05          |
| (1,28)  | 1:16:A:ILE:N   | 1:16:A:ILE:CA   | 1:16:A:ILE:C    | 1:17:A:THR:N   | 8        | 1.05          |
| (1,76)  | 1:42:A:TRP:N   | 1:42:A:TRP:CA   | 1:42:A:TRP:C    | 1:43:A:LYS:N   | 3        | 1.04          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 16       | 1.04          |
| (1,28)  | 1:16:A:ILE:N   | 1:16:A:ILE:CA   | 1:16:A:ILE:C    | 1:17:A:THR:N   | 13       | 1.04          |
| (1,64)  | 1:36:A:THR:N   | 1:36:A:THR:CA   | 1:36:A:THR:C    | 1:37:A:GLU:N   | 12       | 1.03          |
| (1,27)  | 1:15:A:GLY:C   | 1:16:A:ILE:N    | 1:16:A:ILE:CA   | 1:16:A:ILE:C   | 20       | 1.03          |
| (1,131) | 1:1554:A:GLN:N | 1:1554:A:GLN:CA | 1:1554:A:GLN:C  | 1:1555:A:ALA:N | 10       | 1.02          |
| (1,93)  | 1:50:A:ILE:C   | 1:51:A:ASP:N    | 1:51:A:ASP:CA   | 1:51:A:ASP:C   | 19       | 1.02          |
| (1,46)  | 1:25:A:LEU:N   | 1:25:A:LEU:CA   | 1:25:A:LEU:C    | 1:26:A:GLN:N   | 11       | 1.02          |
| (1,27)  | 1:15:A:GLY:C   | 1:16:A:ILE:N    | 1:16:A:ILE:CA   | 1:16:A:ILE:C   | 13       | 1.01          |