



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:22 PM UTC

PDB ID : 2LFV / pdb\_00002lfv  
BMRB ID : 17783  
Title : Solution Structure of the SPOR domain from E. coli DamX  
Authors : Williams, K.B.; Arends, S.J.R.; Popham, D.L.; Fowler, C.A.; Weiss, D.S.  
Deposited on : 2011-07-15

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

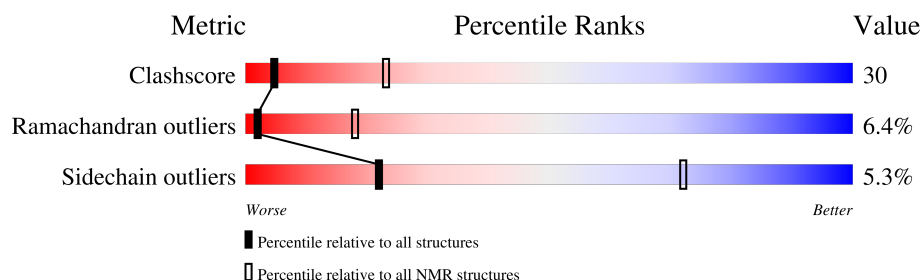
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 96%.

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     | 106    |                  |

## 2 Ensemble composition and analysis

This entry contains 25 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:345-A:424 (80)      | 0.85              | 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 3 clusters and 1 single-model cluster was found.

| Cluster number        | Models                                                              |
|-----------------------|---------------------------------------------------------------------|
| 1                     | 1, 2, 3, 4, 6, 7, 9, 11, 12, 13, 16, 17, 18, 19, 20, 21, 22, 23, 25 |
| 2                     | 8, 10, 15                                                           |
| 3                     | 5, 14                                                               |
| Single-model clusters | 24                                                                  |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1652 atoms, of which 815 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein damX.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 106      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1652  | 522 | 815 | 157 | 157 | 1 |       |

There are 15 discrepancies between the modelled and reference sequences:

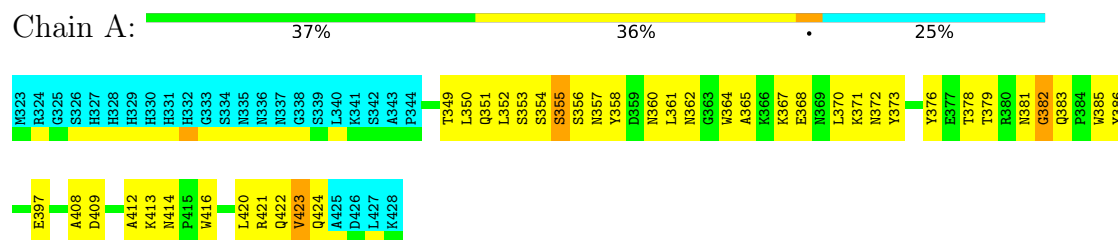
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 323     | MET      | -      | expression tag | UNP P11557 |
| A     | 324     | ARG      | -      | expression tag | UNP P11557 |
| A     | 325     | GLY      | -      | expression tag | UNP P11557 |
| A     | 326     | SER      | -      | expression tag | UNP P11557 |
| A     | 327     | HIS      | -      | expression tag | UNP P11557 |
| A     | 328     | HIS      | -      | expression tag | UNP P11557 |
| A     | 329     | HIS      | -      | expression tag | UNP P11557 |
| A     | 330     | HIS      | -      | expression tag | UNP P11557 |
| A     | 331     | HIS      | -      | expression tag | UNP P11557 |
| A     | 332     | HIS      | -      | expression tag | UNP P11557 |
| A     | 333     | GLY      | -      | expression tag | UNP P11557 |
| A     | 334     | SER      | -      | expression tag | UNP P11557 |
| A     | 335     | ASN      | -      | expression tag | UNP P11557 |
| A     | 336     | ASN      | -      | expression tag | UNP P11557 |
| A     | 337     | ASN      | -      | expression tag | UNP P11557 |

## 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: Protein damX

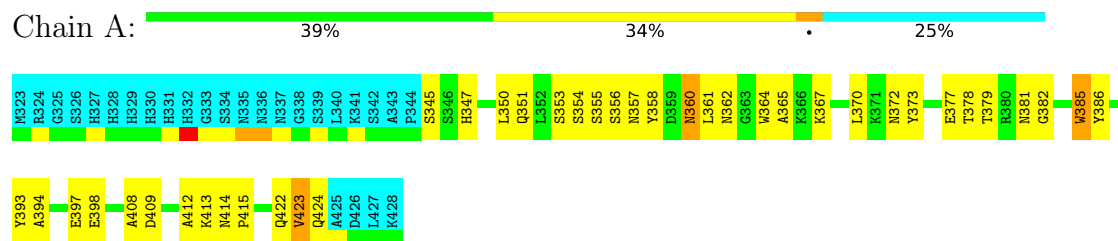


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

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

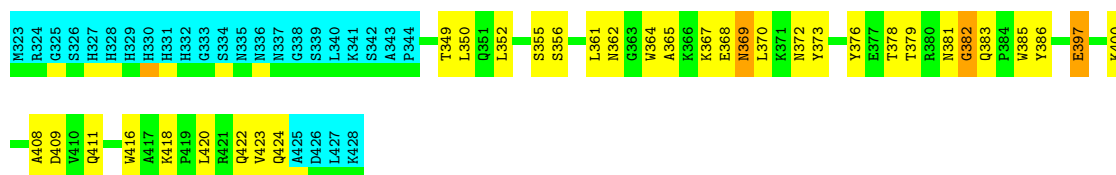
- Molecule 1: Protein damX



#### 4.2.2 Score per residue for model 2

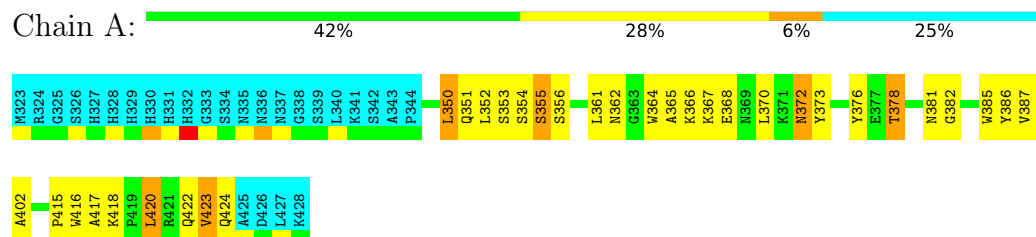
- Molecule 1: Protein damX





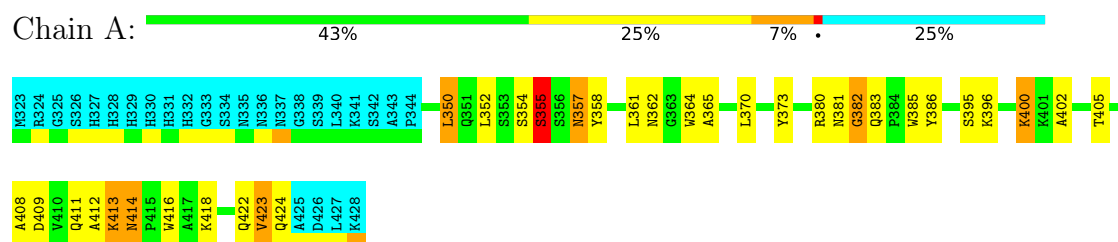
### 4.2.3 Score per residue for model 3

- Molecule 1: Protein damX



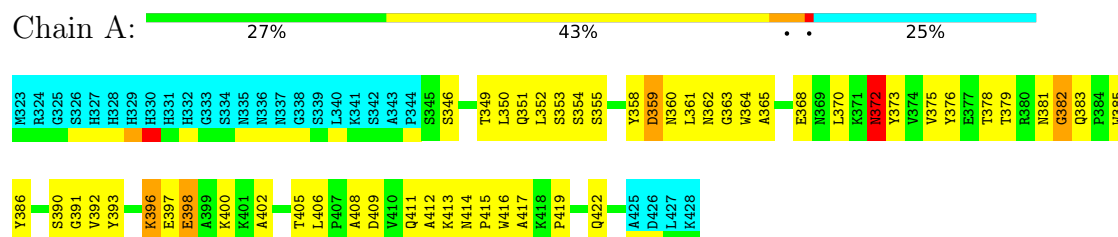
### 4.2.4 Score per residue for model 4

- Molecule 1: Protein damX



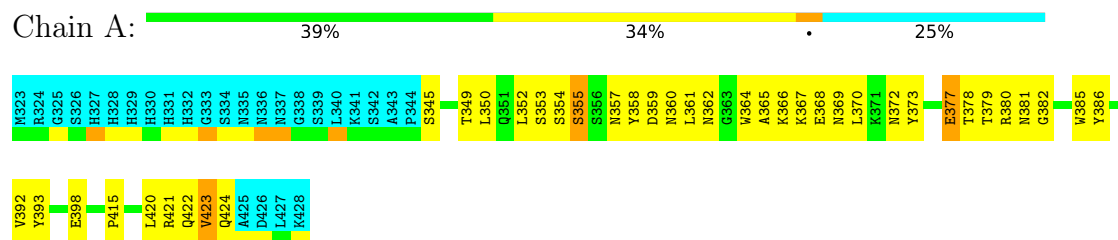
### 4.2.5 Score per residue for model 5

- Molecule 1: Protein damX



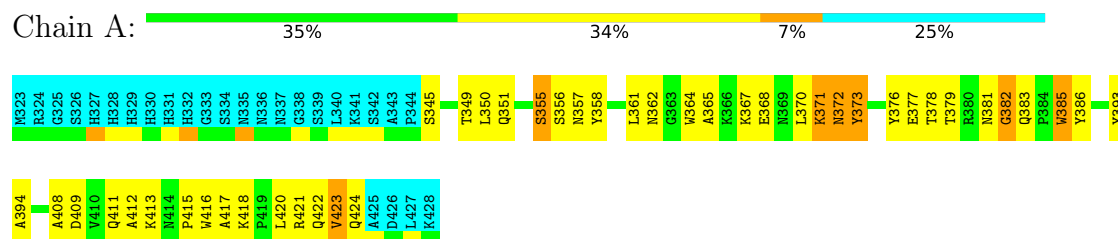
### 4.2.6 Score per residue for model 6

- Molecule 1: Protein damX



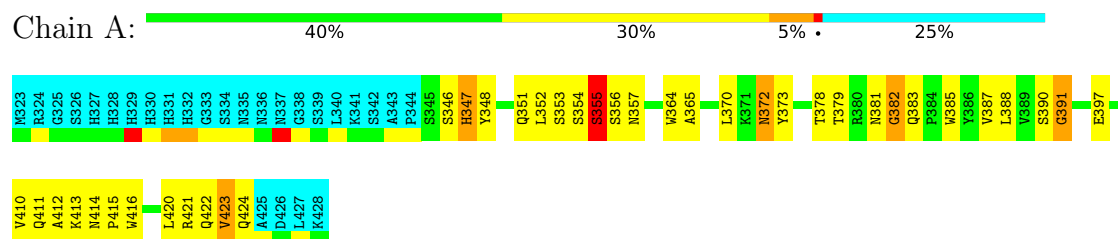
#### 4.2.7 Score per residue for model 7

- Molecule 1: Protein damX



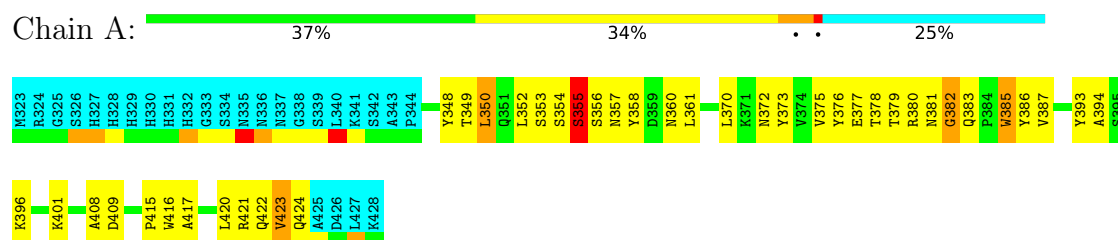
#### 4.2.8 Score per residue for model 8

- Molecule 1: Protein damX



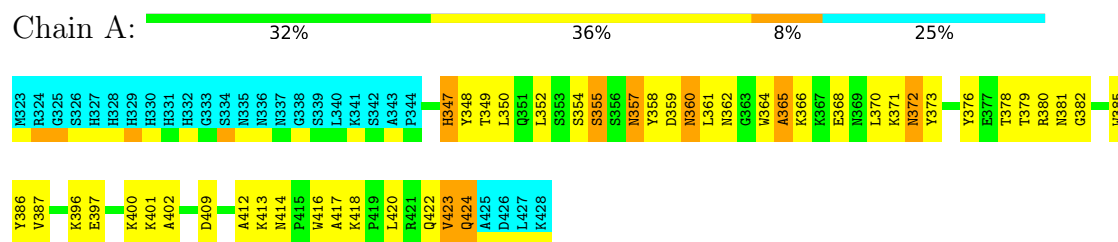
#### 4.2.9 Score per residue for model 9

- Molecule 1: Protein damX



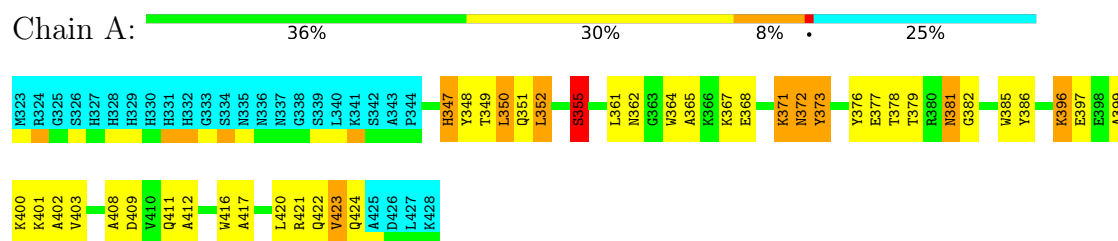
### 4.2.10 Score per residue for model 10

- Molecule 1: Protein damX



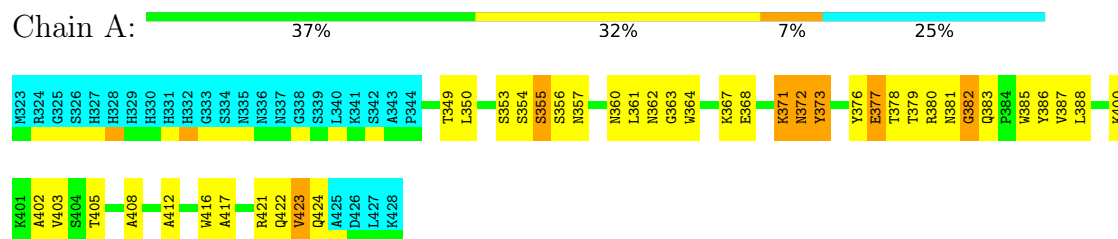
### 4.2.11 Score per residue for model 11

- Molecule 1: Protein damX



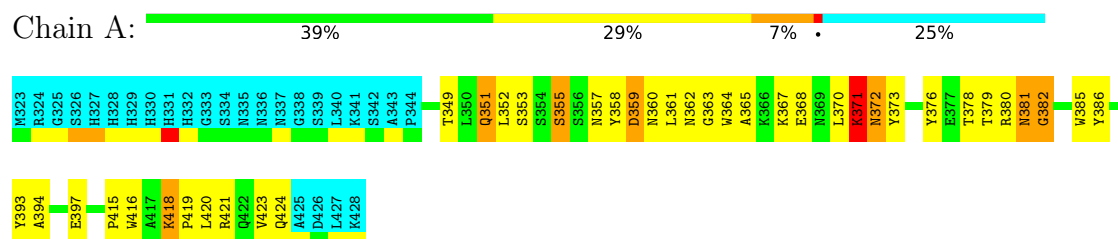
### 4.2.12 Score per residue for model 12

- Molecule 1: Protein damX



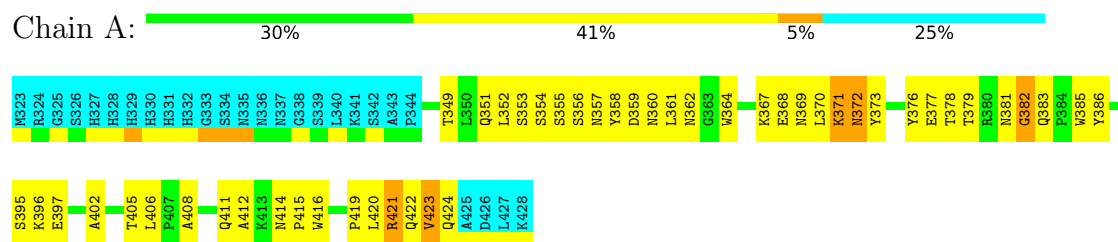
### 4.2.13 Score per residue for model 13

- Molecule 1: Protein damX



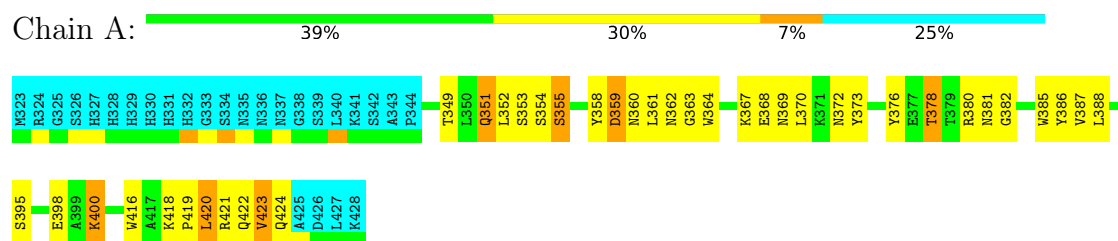
## 4.2.14 Score per residue for model 14

- Molecule 1: Protein damX



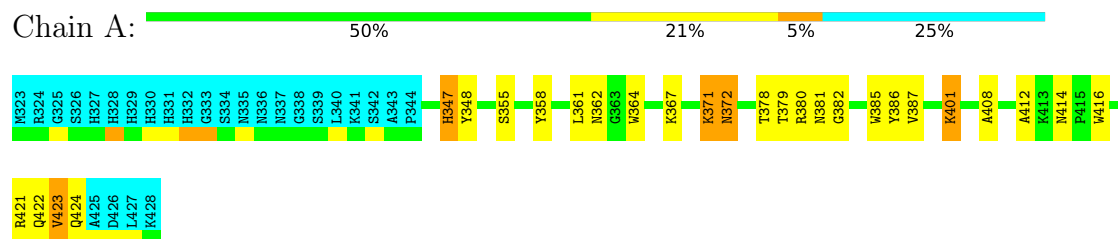
## 4.2.15 Score per residue for model 15

- Molecule 1: Protein damX



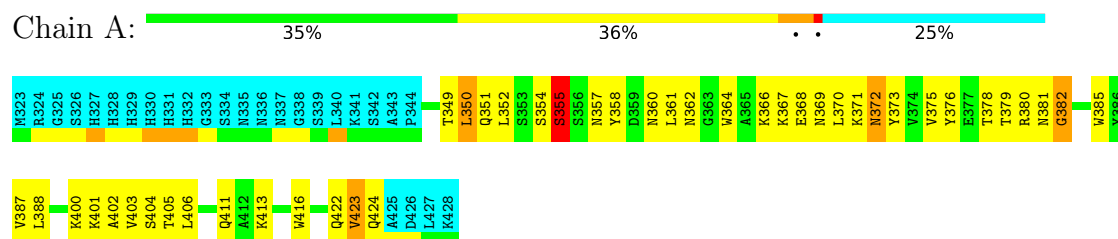
## 4.2.16 Score per residue for model 16

- Molecule 1: Protein damX



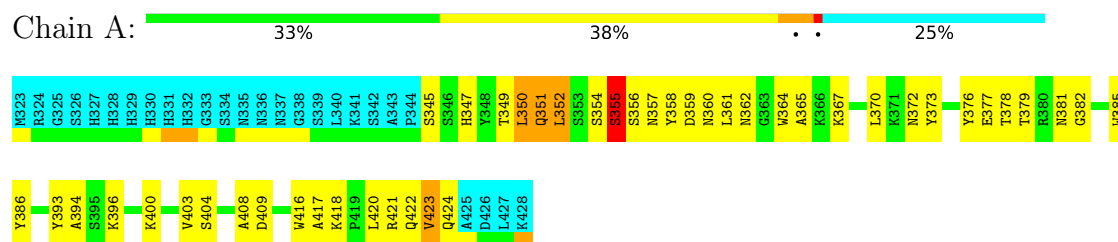
## 4.2.17 Score per residue for model 17

- Molecule 1: Protein damX



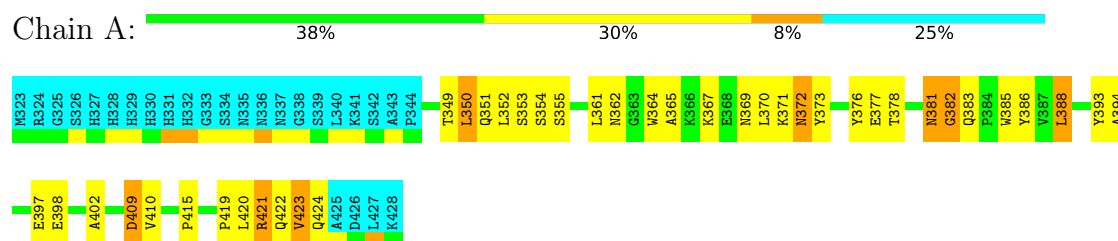
## 4.2.18 Score per residue for model 18

- Molecule 1: Protein damX



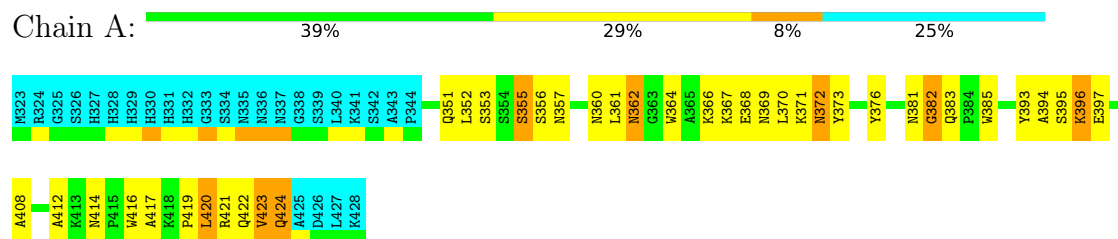
## 4.2.19 Score per residue for model 19

- Molecule 1: Protein damX



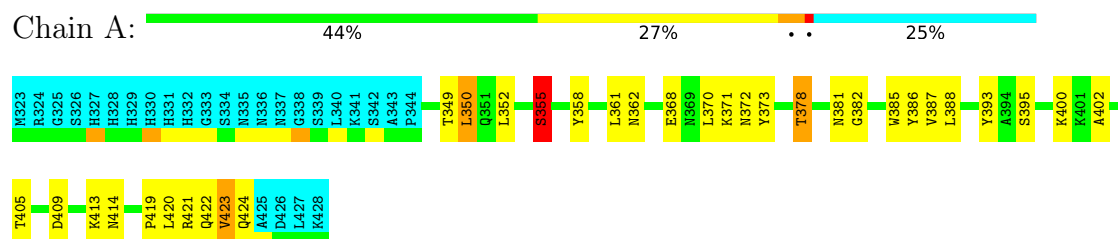
## 4.2.20 Score per residue for model 20

- Molecule 1: Protein damX



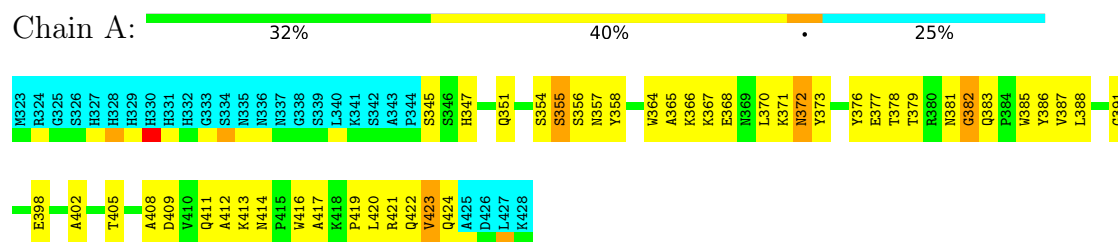
## 4.2.21 Score per residue for model 21

- Molecule 1: Protein damX



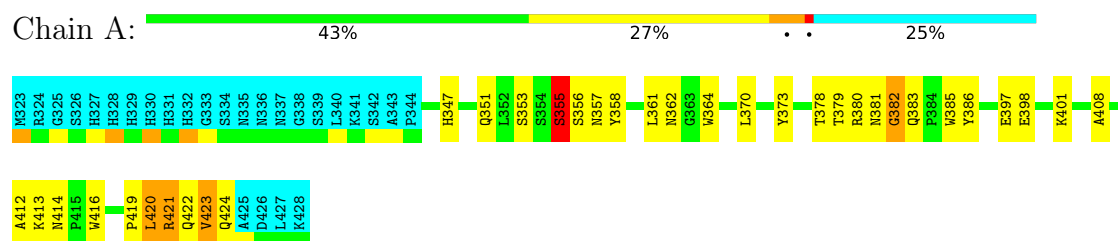
### 4.2.22 Score per residue for model 22

- Molecule 1: Protein damX



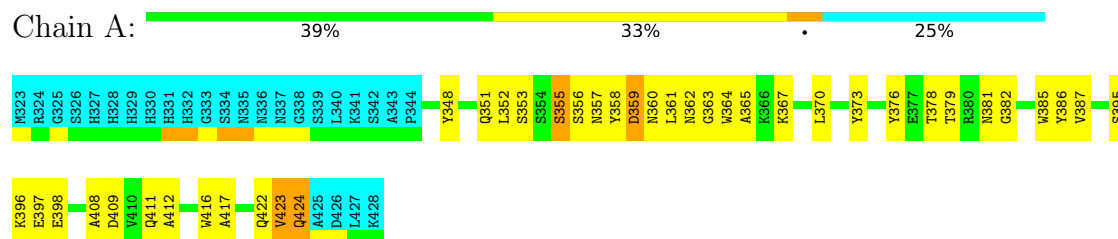
### 4.2.23 Score per residue for model 23

- Molecule 1: Protein damX



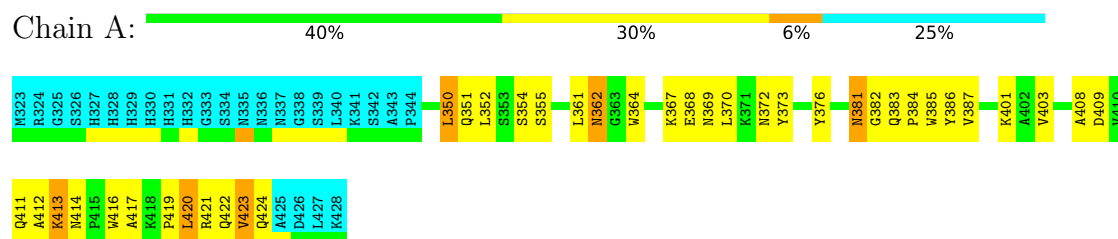
### 4.2.24 Score per residue for model 24

- Molecule 1: Protein damX



### 4.2.25 Score per residue for model 25

- Molecule 1: Protein damX



## 5 Refinement protocol and experimental data overview

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

Of the 250 calculated structures, 25 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| X-PLOR NIH    | structure solution | 2.23    |
| X-PLOR NIH    | refinement         | 2.23    |

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                       | 1284           |
| Number of shifts mapped to atoms             | 1283           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 1              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 96%            |

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 640   | 630      | 629      | 38±6    |
| All | All   | 16000 | 15750    | 15725    | 960     |

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 30.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:352:LEU:N    | 1:A:352:LEU:HD13 | 0.79     | 1.92        | 18     | 1     |
| 1:A:388:LEU:HD22 | 1:A:388:LEU:N    | 0.77     | 1.95        | 19     | 3     |
| 1:A:378:THR:HG22 | 1:A:379:THR:H    | 0.69     | 1.48        | 2      | 4     |
| 1:A:361:LEU:C    | 1:A:361:LEU:HD13 | 0.68     | 2.14        | 16     | 3     |
| 1:A:361:LEU:HD12 | 1:A:385:TRP:CH2  | 0.64     | 2.27        | 21     | 5     |
| 1:A:378:THR:HG22 | 1:A:379:THR:N    | 0.63     | 2.08        | 14     | 4     |
| 1:A:416:TRP:CE2  | 1:A:418:LYS:NZ   | 0.62     | 2.68        | 2      | 1     |
| 1:A:385:TRP:CG   | 1:A:386:TYR:N    | 0.62     | 2.68        | 25     | 10    |
| 1:A:420:LEU:C    | 1:A:420:LEU:HD12 | 0.62     | 2.20        | 13     | 1     |
| 1:A:396:LYS:NZ   | 1:A:400:LYS:NZ   | 0.61     | 2.49        | 18     | 1     |
| 1:A:351:GLN:NE2  | 1:A:380:ARG:NH1  | 0.61     | 2.48        | 23     | 1     |
| 1:A:386:TYR:CD1  | 1:A:386:TYR:N    | 0.60     | 2.69        | 21     | 9     |
| 1:A:352:LEU:N    | 1:A:352:LEU:CD1  | 0.60     | 2.65        | 18     | 7     |
| 1:A:386:TYR:N    | 1:A:386:TYR:CD1  | 0.59     | 2.70        | 25     | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:402:ALA:O    | 1:A:405:THR:HG22 | 0.59     | 1.97        | 4      | 3     |
| 1:A:355:SER:N    | 1:A:380:ARG:HH12 | 0.58     | 1.96        | 9      | 1     |
| 1:A:354:SER:H    | 1:A:413:LYS:HZ2  | 0.57     | 1.40        | 8      | 1     |
| 1:A:352:LEU:HD12 | 1:A:352:LEU:N    | 0.57     | 2.14        | 24     | 6     |
| 1:A:372:ASN:HD22 | 1:A:372:ASN:N    | 0.57     | 1.96        | 16     | 1     |
| 1:A:388:LEU:N    | 1:A:388:LEU:CD2  | 0.57     | 2.67        | 19     | 3     |
| 1:A:385:TRP:CD2  | 1:A:386:TYR:N    | 0.56     | 2.73        | 12     | 11    |
| 1:A:351:GLN:NE2  | 1:A:380:ARG:HH22 | 0.56     | 1.98        | 17     | 1     |
| 1:A:358:TYR:CE1  | 1:A:362:ASN:ND2  | 0.56     | 2.74        | 23     | 3     |
| 1:A:352:LEU:HD22 | 1:A:352:LEU:N    | 0.55     | 2.16        | 19     | 1     |
| 1:A:355:SER:OG   | 1:A:356:SER:N    | 0.55     | 2.40        | 22     | 3     |
| 1:A:421:ARG:NH2  | 1:A:422:GLN:NE2  | 0.55     | 2.55        | 12     | 1     |
| 1:A:381:ASN:HD22 | 1:A:381:ASN:N    | 0.55     | 1.98        | 25     | 2     |
| 1:A:355:SER:O    | 1:A:385:TRP:CE3  | 0.55     | 2.60        | 12     | 23    |
| 1:A:396:LYS:HZ2  | 1:A:400:LYS:HZ2  | 0.55     | 1.45        | 18     | 1     |
| 1:A:377:GLU:H    | 1:A:377:GLU:CD   | 0.55     | 2.10        | 19     | 3     |
| 1:A:361:LEU:HD22 | 1:A:385:TRP:CH2  | 0.55     | 2.37        | 12     | 7     |
| 1:A:396:LYS:HZ2  | 1:A:400:LYS:NZ   | 0.54     | 2.00        | 18     | 1     |
| 1:A:422:GLN:C    | 1:A:424:GLN:N    | 0.54     | 2.65        | 20     | 23    |
| 1:A:355:SER:OG   | 1:A:385:TRP:CH2  | 0.54     | 2.60        | 4      | 1     |
| 1:A:420:LEU:N    | 1:A:420:LEU:HD12 | 0.54     | 2.17        | 10     | 1     |
| 1:A:422:GLN:O    | 1:A:424:GLN:N    | 0.54     | 2.41        | 19     | 22    |
| 1:A:416:TRP:CD1  | 1:A:416:TRP:N    | 0.54     | 2.75        | 4      | 7     |
| 1:A:353:SER:OG   | 1:A:364:TRP:CH2  | 0.54     | 2.60        | 23     | 2     |
| 1:A:370:LEU:O    | 1:A:373:TYR:CE1  | 0.54     | 2.61        | 25     | 18    |
| 1:A:420:LEU:CD2  | 1:A:420:LEU:N    | 0.54     | 2.71        | 8      | 2     |
| 1:A:388:LEU:N    | 1:A:388:LEU:CD1  | 0.54     | 2.71        | 15     | 1     |
| 1:A:351:GLN:HE22 | 1:A:380:ARG:NH1  | 0.54     | 2.01        | 17     | 1     |
| 1:A:351:GLN:OE1  | 1:A:353:SER:N    | 0.54     | 2.41        | 24     | 4     |
| 1:A:395:SER:O    | 1:A:397:GLU:N    | 0.53     | 2.41        | 20     | 1     |
| 1:A:370:LEU:O    | 1:A:373:TYR:CD1  | 0.53     | 2.62        | 24     | 15    |
| 1:A:347:HIS:O    | 1:A:348:TYR:CD2  | 0.53     | 2.61        | 8      | 4     |
| 1:A:388:LEU:N    | 1:A:388:LEU:HD12 | 0.53     | 2.17        | 15     | 1     |
| 1:A:398:GLU:CD   | 1:A:398:GLU:H    | 0.53     | 2.10        | 15     | 3     |
| 1:A:420:LEU:N    | 1:A:420:LEU:HD22 | 0.53     | 2.17        | 8      | 2     |
| 1:A:364:TRP:CD1  | 1:A:368:GLU:OE1  | 0.53     | 2.62        | 25     | 8     |
| 1:A:352:LEU:N    | 1:A:352:LEU:CD2  | 0.53     | 2.71        | 19     | 1     |
| 1:A:354:SER:OG   | 1:A:380:ARG:NH1  | 0.53     | 2.42        | 9      | 1     |
| 1:A:364:TRP:O    | 1:A:367:LYS:N    | 0.53     | 2.42        | 22     | 13    |
| 1:A:364:TRP:CZ2  | 1:A:368:GLU:OE1  | 0.53     | 2.62        | 12     | 4     |
| 1:A:381:ASN:O    | 1:A:383:GLN:N    | 0.53     | 2.42        | 12     | 12    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:351:GLN:NE2  | 1:A:353:SER:C    | 0.53     | 2.67        | 3      | 2     |
| 1:A:352:LEU:CD1  | 1:A:352:LEU:N    | 0.53     | 2.72        | 6      | 3     |
| 1:A:372:ASN:O    | 1:A:372:ASN:ND2  | 0.53     | 2.42        | 12     | 5     |
| 1:A:372:ASN:N    | 1:A:372:ASN:ND2  | 0.53     | 2.53        | 16     | 1     |
| 1:A:416:TRP:CE3  | 1:A:417:ALA:O    | 0.53     | 2.62        | 9      | 12    |
| 1:A:355:SER:O    | 1:A:385:TRP:CD2  | 0.53     | 2.61        | 17     | 7     |
| 1:A:355:SER:O    | 1:A:380:ARG:NH1  | 0.53     | 2.42        | 9      | 1     |
| 1:A:351:GLN:OE1  | 1:A:416:TRP:NE1  | 0.53     | 2.42        | 20     | 1     |
| 1:A:351:GLN:NE2  | 1:A:353:SER:O    | 0.52     | 2.43        | 1      | 1     |
| 1:A:364:TRP:CZ2  | 1:A:368:GLU:CD   | 0.52     | 2.87        | 10     | 4     |
| 1:A:380:ARG:NH1  | 1:A:381:ASN:ND2  | 0.52     | 2.57        | 6      | 2     |
| 1:A:376:TYR:CE2  | 1:A:378:THR:OG1  | 0.52     | 2.62        | 2      | 2     |
| 1:A:355:SER:C    | 1:A:385:TRP:CE3  | 0.52     | 2.87        | 23     | 10    |
| 1:A:358:TYR:O    | 1:A:361:LEU:N    | 0.52     | 2.41        | 10     | 6     |
| 1:A:411:GLN:O    | 1:A:414:ASN:N    | 0.52     | 2.42        | 14     | 3     |
| 1:A:364:TRP:NE1  | 1:A:368:GLU:OE1  | 0.52     | 2.42        | 25     | 3     |
| 1:A:385:TRP:CE2  | 1:A:386:TYR:O    | 0.52     | 2.63        | 23     | 4     |
| 1:A:360:ASN:N    | 1:A:360:ASN:OD1  | 0.52     | 2.42        | 10     | 1     |
| 1:A:360:ASN:OD1  | 1:A:361:LEU:N    | 0.52     | 2.42        | 12     | 1     |
| 1:A:351:GLN:HE22 | 1:A:353:SER:CA   | 0.52     | 2.17        | 24     | 1     |
| 1:A:350:LEU:N    | 1:A:350:LEU:CD2  | 0.52     | 2.72        | 2      | 7     |
| 1:A:356:SER:OG   | 1:A:380:ARG:NH2  | 0.52     | 2.42        | 9      | 1     |
| 1:A:377:GLU:CD   | 1:A:377:GLU:N    | 0.52     | 2.67        | 12     | 1     |
| 1:A:385:TRP:CZ2  | 1:A:386:TYR:O    | 0.52     | 2.63        | 25     | 10    |
| 1:A:395:SER:OG   | 1:A:396:LYS:N    | 0.52     | 2.41        | 24     | 3     |
| 1:A:358:TYR:O    | 1:A:360:ASN:N    | 0.52     | 2.43        | 5      | 7     |
| 1:A:377:GLU:OE1  | 1:A:377:GLU:N    | 0.52     | 2.43        | 9      | 1     |
| 1:A:402:ALA:O    | 1:A:405:THR:N    | 0.52     | 2.42        | 21     | 2     |
| 1:A:364:TRP:CH2  | 1:A:368:GLU:OE1  | 0.52     | 2.62        | 17     | 1     |
| 1:A:408:ALA:O    | 1:A:412:ALA:N    | 0.52     | 2.42        | 25     | 12    |
| 1:A:359:ASP:O    | 1:A:362:ASN:ND2  | 0.52     | 2.42        | 5      | 4     |
| 1:A:349:THR:HG23 | 1:A:349:THR:O    | 0.52     | 2.05        | 2      | 5     |
| 1:A:408:ALA:O    | 1:A:411:GLN:N    | 0.52     | 2.42        | 22     | 6     |
| 1:A:357:ASN:ND2  | 1:A:360:ASN:OD1  | 0.52     | 2.43        | 13     | 2     |
| 1:A:378:THR:OG1  | 1:A:379:THR:N    | 0.52     | 2.43        | 9      | 8     |
| 1:A:364:TRP:NE1  | 1:A:368:GLU:CD   | 0.52     | 2.67        | 13     | 4     |
| 1:A:358:TYR:C    | 1:A:360:ASN:N    | 0.52     | 2.66        | 5      | 8     |
| 1:A:398:GLU:CD   | 1:A:398:GLU:N    | 0.52     | 2.68        | 5      | 2     |
| 1:A:351:GLN:NE2  | 1:A:416:TRP:HE1  | 0.52     | 2.03        | 3      | 2     |
| 1:A:350:LEU:N    | 1:A:350:LEU:HD22 | 0.51     | 2.20        | 2      | 7     |
| 1:A:350:LEU:HD12 | 1:A:350:LEU:N    | 0.51     | 2.20        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:421:ARG:NE   | 1:A:421:ARG:C    | 0.51     | 2.68        | 12     | 1     |
| 1:A:420:LEU:C    | 1:A:422:GLN:N    | 0.51     | 2.67        | 23     | 5     |
| 1:A:351:GLN:NE2  | 1:A:354:SER:OG   | 0.51     | 2.44        | 17     | 1     |
| 1:A:414:ASN:O    | 1:A:414:ASN:ND2  | 0.51     | 2.43        | 1      | 2     |
| 1:A:368:GLU:CD   | 1:A:368:GLU:N    | 0.51     | 2.67        | 13     | 3     |
| 1:A:385:TRP:CE3  | 1:A:386:TYR:N    | 0.51     | 2.79        | 14     | 5     |
| 1:A:395:SER:N    | 1:A:398:GLU:OE2  | 0.51     | 2.43        | 15     | 1     |
| 1:A:353:SER:OG   | 1:A:354:SER:N    | 0.51     | 2.44        | 3      | 9     |
| 1:A:352:LEU:N    | 1:A:352:LEU:HD12 | 0.51     | 2.21        | 4      | 3     |
| 1:A:354:SER:H    | 1:A:413:LYS:NZ   | 0.51     | 2.04        | 8      | 2     |
| 1:A:351:GLN:NE2  | 1:A:351:GLN:C    | 0.51     | 2.68        | 11     | 1     |
| 1:A:351:GLN:CD   | 1:A:352:LEU:N    | 0.51     | 2.68        | 11     | 1     |
| 1:A:419:PRO:C    | 1:A:421:ARG:N    | 0.51     | 2.68        | 22     | 8     |
| 1:A:364:TRP:CH2  | 1:A:368:GLU:OE2  | 0.51     | 2.64        | 6      | 1     |
| 1:A:364:TRP:CE2  | 1:A:368:GLU:CD   | 0.51     | 2.89        | 10     | 1     |
| 1:A:421:ARG:NE   | 1:A:421:ARG:O    | 0.51     | 2.44        | 12     | 1     |
| 1:A:359:ASP:C    | 1:A:362:ASN:ND2  | 0.50     | 2.69        | 15     | 4     |
| 1:A:362:ASN:C    | 1:A:362:ASN:HD22 | 0.50     | 2.14        | 20     | 1     |
| 1:A:378:THR:HG23 | 1:A:379:THR:N    | 0.50     | 2.21        | 7      | 4     |
| 1:A:420:LEU:O    | 1:A:422:GLN:N    | 0.50     | 2.45        | 19     | 4     |
| 1:A:364:TRP:CZ2  | 1:A:368:GLU:OE2  | 0.50     | 2.65        | 6      | 2     |
| 1:A:381:ASN:N    | 1:A:381:ASN:OD1  | 0.50     | 2.43        | 11     | 1     |
| 1:A:351:GLN:CD   | 1:A:416:TRP:HE1  | 0.50     | 2.15        | 25     | 3     |
| 1:A:421:ARG:C    | 1:A:421:ARG:HE   | 0.50     | 2.14        | 12     | 1     |
| 1:A:376:TYR:N    | 1:A:376:TYR:CD1  | 0.50     | 2.79        | 20     | 7     |
| 1:A:387:VAL:HG11 | 1:A:418:LYS:HZ2  | 0.50     | 1.65        | 3      | 1     |
| 1:A:375:VAL:HG23 | 1:A:375:VAL:O    | 0.50     | 2.07        | 17     | 3     |
| 1:A:352:LEU:HD13 | 1:A:352:LEU:H    | 0.50     | 1.64        | 18     | 1     |
| 1:A:373:TYR:CD1  | 1:A:373:TYR:C    | 0.49     | 2.90        | 12     | 2     |
| 1:A:362:ASN:C    | 1:A:362:ASN:ND2  | 0.49     | 2.70        | 20     | 1     |
| 1:A:357:ASN:N    | 1:A:357:ASN:ND2  | 0.49     | 2.59        | 10     | 1     |
| 1:A:368:GLU:N    | 1:A:368:GLU:CD   | 0.49     | 2.70        | 3      | 4     |
| 1:A:422:GLN:O    | 1:A:423:VAL:C    | 0.49     | 2.56        | 25     | 13    |
| 1:A:390:SER:OG   | 1:A:391:GLY:N    | 0.49     | 2.42        | 8      | 1     |
| 1:A:355:SER:H    | 1:A:380:ARG:NH1  | 0.49     | 2.05        | 9      | 1     |
| 1:A:381:ASN:C    | 1:A:383:GLN:N    | 0.49     | 2.70        | 12     | 11    |
| 1:A:357:ASN:N    | 1:A:357:ASN:OD1  | 0.49     | 2.43        | 17     | 1     |
| 1:A:387:VAL:C    | 1:A:388:LEU:HD12 | 0.49     | 2.33        | 21     | 1     |
| 1:A:359:ASP:C    | 1:A:362:ASN:HD21 | 0.49     | 2.16        | 15     | 2     |
| 1:A:380:ARG:NH2  | 1:A:416:TRP:CZ2  | 0.49     | 2.81        | 12     | 1     |
| 1:A:387:VAL:HG11 | 1:A:418:LYS:NZ   | 0.48     | 2.23        | 3      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:420:LEU:HD23 | 1:A:420:LEU:O    | 0.48     | 2.08        | 3      | 4     |
| 1:A:420:LEU:HD12 | 1:A:421:ARG:N    | 0.48     | 2.22        | 13     | 1     |
| 1:A:381:ASN:N    | 1:A:381:ASN:ND2  | 0.48     | 2.60        | 13     | 2     |
| 1:A:400:LYS:C    | 1:A:402:ALA:N    | 0.48     | 2.69        | 5      | 2     |
| 1:A:355:SER:N    | 1:A:380:ARG:NH1  | 0.48     | 2.60        | 9      | 1     |
| 1:A:350:LEU:N    | 1:A:350:LEU:CD1  | 0.48     | 2.76        | 9      | 1     |
| 1:A:361:LEU:C    | 1:A:361:LEU:CD1  | 0.48     | 2.86        | 15     | 3     |
| 1:A:361:LEU:O    | 1:A:361:LEU:HD23 | 0.48     | 2.09        | 20     | 1     |
| 1:A:351:GLN:NE2  | 1:A:380:ARG:CZ   | 0.48     | 2.77        | 23     | 1     |
| 1:A:411:GLN:C    | 1:A:413:LYS:N    | 0.48     | 2.71        | 17     | 1     |
| 1:A:395:SER:C    | 1:A:397:GLU:N    | 0.48     | 2.68        | 20     | 1     |
| 1:A:419:PRO:O    | 1:A:421:ARG:N    | 0.48     | 2.47        | 22     | 3     |
| 1:A:368:GLU:CD   | 1:A:370:LEU:HD21 | 0.48     | 2.34        | 6      | 1     |
| 1:A:376:TYR:CE1  | 1:A:387:VAL:O    | 0.48     | 2.67        | 12     | 4     |
| 1:A:360:ASN:N    | 1:A:360:ASN:ND2  | 0.48     | 2.59        | 13     | 1     |
| 1:A:347:HIS:O    | 1:A:420:LEU:CD1  | 0.48     | 2.62        | 23     | 1     |
| 1:A:396:LYS:NZ   | 1:A:396:LYS:CB   | 0.48     | 2.77        | 5      | 3     |
| 1:A:371:LYS:O    | 1:A:372:ASN:C    | 0.48     | 2.57        | 7      | 7     |
| 1:A:388:LEU:CD2  | 1:A:388:LEU:N    | 0.47     | 2.76        | 3      | 1     |
| 1:A:361:LEU:HD23 | 1:A:361:LEU:C    | 0.47     | 2.34        | 20     | 2     |
| 1:A:373:TYR:C    | 1:A:373:TYR:CD1  | 0.47     | 2.90        | 7      | 1     |
| 1:A:376:TYR:CD2  | 1:A:377:GLU:O    | 0.47     | 2.67        | 7      | 4     |
| 1:A:420:LEU:C    | 1:A:420:LEU:CD1  | 0.47     | 2.87        | 13     | 1     |
| 1:A:361:LEU:C    | 1:A:361:LEU:HD23 | 0.47     | 2.34        | 10     | 1     |
| 1:A:351:GLN:CD   | 1:A:380:ARG:HH22 | 0.47     | 2.18        | 17     | 1     |
| 1:A:356:SER:O    | 1:A:357:ASN:ND2  | 0.47     | 2.48        | 1      | 1     |
| 1:A:378:THR:CG2  | 1:A:379:THR:N    | 0.47     | 2.78        | 2      | 4     |
| 1:A:397:GLU:CG   | 1:A:398:GLU:N    | 0.47     | 2.77        | 1      | 3     |
| 1:A:410:VAL:C    | 1:A:412:ALA:N    | 0.47     | 2.70        | 8      | 1     |
| 1:A:360:ASN:N    | 1:A:360:ASN:HD22 | 0.47     | 2.06        | 13     | 1     |
| 1:A:367:LYS:C    | 1:A:369:ASN:N    | 0.47     | 2.72        | 14     | 4     |
| 1:A:378:THR:N    | 1:A:385:TRP:O    | 0.47     | 2.46        | 21     | 4     |
| 1:A:362:ASN:OD1  | 1:A:363:GLY:N    | 0.47     | 2.48        | 5      | 2     |
| 1:A:372:ASN:C    | 1:A:372:ASN:ND2  | 0.47     | 2.71        | 10     | 1     |
| 1:A:351:GLN:C    | 1:A:352:LEU:HD22 | 0.47     | 2.35        | 5      | 1     |
| 1:A:367:LYS:O    | 1:A:369:ASN:ND2  | 0.47     | 2.46        | 20     | 2     |
| 1:A:422:GLN:C    | 1:A:424:GLN:H    | 0.47     | 2.18        | 10     | 7     |
| 1:A:398:GLU:N    | 1:A:398:GLU:OE1  | 0.47     | 2.48        | 5      | 1     |
| 1:A:368:GLU:CD   | 1:A:368:GLU:H    | 0.47     | 2.17        | 14     | 1     |
| 1:A:358:TYR:CD1  | 1:A:358:TYR:C    | 0.46     | 2.94        | 1      | 9     |
| 1:A:398:GLU:O    | 1:A:402:ALA:N    | 0.46     | 2.47        | 3      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:351:GLN:C    | 1:A:352:LEU:HD12 | 0.46     | 2.34        | 14     | 1     |
| 1:A:388:LEU:N    | 1:A:388:LEU:HD22 | 0.46     | 2.25        | 3      | 1     |
| 1:A:412:ALA:C    | 1:A:414:ASN:H    | 0.46     | 2.18        | 16     | 4     |
| 1:A:358:TYR:CE1  | 1:A:362:ASN:OD1  | 0.46     | 2.69        | 7      | 1     |
| 1:A:419:PRO:C    | 1:A:421:ARG:H    | 0.46     | 2.17        | 15     | 2     |
| 1:A:351:GLN:NE2  | 1:A:380:ARG:HH12 | 0.46     | 2.09        | 17     | 1     |
| 1:A:420:LEU:C    | 1:A:422:GLN:H    | 0.46     | 2.19        | 21     | 3     |
| 1:A:358:TYR:C    | 1:A:360:ASN:H    | 0.46     | 2.19        | 14     | 4     |
| 1:A:377:GLU:CG   | 1:A:378:THR:N    | 0.46     | 2.78        | 18     | 3     |
| 1:A:354:SER:N    | 1:A:413:LYS:HZ2  | 0.46     | 2.08        | 8      | 1     |
| 1:A:351:GLN:NE2  | 1:A:352:LEU:N    | 0.46     | 2.63        | 11     | 1     |
| 1:A:364:TRP:CE2  | 1:A:368:GLU:OE1  | 0.46     | 2.69        | 13     | 2     |
| 1:A:372:ASN:C    | 1:A:372:ASN:HD22 | 0.46     | 2.19        | 5      | 1     |
| 1:A:355:SER:O    | 1:A:385:TRP:CG   | 0.46     | 2.69        | 10     | 1     |
| 1:A:354:SER:H    | 1:A:413:LYS:HZ3  | 0.46     | 1.52        | 22     | 1     |
| 1:A:378:THR:CG2  | 1:A:379:THR:H    | 0.46     | 2.22        | 14     | 4     |
| 1:A:400:LYS:CB   | 1:A:400:LYS:NZ   | 0.46     | 2.77        | 21     | 2     |
| 1:A:351:GLN:OE1  | 1:A:416:TRP:CD1  | 0.46     | 2.68        | 20     | 1     |
| 1:A:381:ASN:O    | 1:A:382:GLY:C    | 0.46     | 2.59        | 19     | 25    |
| 1:A:403:VAL:CG1  | 1:A:411:GLN:CD   | 0.45     | 2.89        | 11     | 1     |
| 1:A:361:LEU:O    | 1:A:365:ALA:N    | 0.45     | 2.48        | 18     | 1     |
| 1:A:351:GLN:HE22 | 1:A:380:ARG:NH2  | 0.45     | 2.08        | 23     | 1     |
| 1:A:345:SER:OG   | 1:A:421:ARG:N    | 0.45     | 2.50        | 7      | 1     |
| 1:A:357:ASN:O    | 1:A:357:ASN:ND2  | 0.45     | 2.49        | 4      | 1     |
| 1:A:420:LEU:H    | 1:A:420:LEU:HD12 | 0.45     | 1.72        | 23     | 1     |
| 1:A:360:ASN:C    | 1:A:360:ASN:HD22 | 0.45     | 2.18        | 1      | 1     |
| 1:A:361:LEU:HD12 | 1:A:385:TRP:CZ2  | 0.45     | 2.46        | 23     | 3     |
| 1:A:351:GLN:HE22 | 1:A:380:ARG:CZ   | 0.45     | 2.24        | 23     | 1     |
| 1:A:367:LYS:C    | 1:A:369:ASN:H    | 0.45     | 2.20        | 14     | 2     |
| 1:A:380:ARG:NH2  | 1:A:418:LYS:NZ   | 0.45     | 2.64        | 15     | 2     |
| 1:A:403:VAL:C    | 1:A:405:THR:H    | 0.45     | 2.20        | 17     | 2     |
| 1:A:357:ASN:ND2  | 1:A:360:ASN:CG   | 0.45     | 2.74        | 13     | 2     |
| 1:A:401:LYS:CB   | 1:A:401:LYS:NZ   | 0.45     | 2.79        | 16     | 1     |
| 1:A:351:GLN:OE1  | 1:A:351:GLN:C    | 0.45     | 2.60        | 13     | 3     |
| 1:A:413:LYS:CD   | 1:A:413:LYS:H    | 0.45     | 2.25        | 4      | 1     |
| 1:A:363:GLY:O    | 1:A:367:LYS:N    | 0.45     | 2.48        | 12     | 1     |
| 1:A:358:TYR:C    | 1:A:358:TYR:CD1  | 0.45     | 2.95        | 24     | 3     |
| 1:A:376:TYR:CD1  | 1:A:376:TYR:N    | 0.45     | 2.85        | 25     | 2     |
| 1:A:349:THR:O    | 1:A:350:LEU:HD22 | 0.44     | 2.12        | 10     | 2     |
| 1:A:409:ASP:OD1  | 1:A:409:ASP:N    | 0.44     | 2.50        | 5      | 1     |
| 1:A:418:LYS:NZ   | 1:A:418:LYS:CB   | 0.44     | 2.80        | 13     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:351:GLN:OE1  | 1:A:351:GLN:O    | 0.44     | 2.35        | 15     | 1     |
| 1:A:393:TYR:C    | 1:A:395:SER:N    | 0.44     | 2.74        | 21     | 1     |
| 1:A:385:TRP:NE1  | 1:A:387:VAL:HG22 | 0.44     | 2.27        | 10     | 1     |
| 1:A:365:ALA:O    | 1:A:366:LYS:C    | 0.44     | 2.60        | 10     | 1     |
| 1:A:405:THR:HG23 | 1:A:406:LEU:N    | 0.44     | 2.25        | 17     | 1     |
| 1:A:411:GLN:C    | 1:A:413:LYS:H    | 0.44     | 2.19        | 17     | 1     |
| 1:A:369:ASN:C    | 1:A:369:ASN:HD22 | 0.44     | 2.19        | 2      | 1     |
| 1:A:351:GLN:HE22 | 1:A:380:ARG:HH12 | 0.44     | 1.54        | 17     | 1     |
| 1:A:372:ASN:ND2  | 1:A:372:ASN:O    | 0.44     | 2.49        | 16     | 1     |
| 1:A:420:LEU:C    | 1:A:424:GLN:HE21 | 0.44     | 2.21        | 23     | 1     |
| 1:A:351:GLN:NE2  | 1:A:380:ARG:NH2  | 0.44     | 2.64        | 17     | 1     |
| 1:A:361:LEU:O    | 1:A:362:ASN:C    | 0.44     | 2.61        | 4      | 13    |
| 1:A:351:GLN:O    | 1:A:351:GLN:OE1  | 0.44     | 2.36        | 3      | 2     |
| 1:A:345:SER:CB   | 1:A:424:GLN:HE22 | 0.44     | 2.25        | 6      | 1     |
| 1:A:390:SER:O    | 1:A:391:GLY:O    | 0.44     | 2.36        | 8      | 1     |
| 1:A:408:ALA:O    | 1:A:409:ASP:C    | 0.44     | 2.61        | 24     | 9     |
| 1:A:364:TRP:O    | 1:A:365:ALA:C    | 0.43     | 2.61        | 19     | 13    |
| 1:A:349:THR:O    | 1:A:350:LEU:O    | 0.43     | 2.36        | 19     | 2     |
| 1:A:362:ASN:CG   | 1:A:363:GLY:N    | 0.43     | 2.75        | 15     | 3     |
| 1:A:357:ASN:O    | 1:A:360:ASN:OD1  | 0.43     | 2.36        | 12     | 1     |
| 1:A:357:ASN:ND2  | 1:A:360:ASN:ND2  | 0.43     | 2.66        | 13     | 1     |
| 1:A:345:SER:C    | 1:A:347:HIS:N    | 0.43     | 2.75        | 1      | 3     |
| 1:A:371:LYS:O    | 1:A:372:ASN:O    | 0.43     | 2.37        | 14     | 2     |
| 1:A:351:GLN:CG   | 1:A:353:SER:O    | 0.43     | 2.66        | 20     | 1     |
| 1:A:356:SER:O    | 1:A:357:ASN:CG   | 0.43     | 2.61        | 8      | 11    |
| 1:A:362:ASN:O    | 1:A:366:LYS:CG   | 0.43     | 2.66        | 3      | 2     |
| 1:A:409:ASP:N    | 1:A:409:ASP:OD1  | 0.43     | 2.50        | 10     | 1     |
| 1:A:371:LYS:O    | 1:A:373:TYR:N    | 0.43     | 2.51        | 12     | 1     |
| 1:A:371:LYS:O    | 1:A:372:ASN:CG   | 0.43     | 2.61        | 19     | 3     |
| 1:A:401:LYS:O    | 1:A:404:SER:N    | 0.43     | 2.50        | 17     | 1     |
| 1:A:413:LYS:O    | 1:A:414:ASN:CG   | 0.43     | 2.62        | 5      | 2     |
| 1:A:364:TRP:O    | 1:A:368:GLU:OE1  | 0.43     | 2.37        | 20     | 3     |
| 1:A:387:VAL:HG22 | 1:A:388:LEU:N    | 0.43     | 2.28        | 17     | 2     |
| 1:A:380:ARG:NH1  | 1:A:381:ASN:OD1  | 0.43     | 2.51        | 10     | 1     |
| 1:A:352:LEU:O    | 1:A:353:SER:OG   | 0.43     | 2.36        | 13     | 1     |
| 1:A:380:ARG:C    | 1:A:381:ASN:HD22 | 0.43     | 2.20        | 13     | 1     |
| 1:A:416:TRP:CZ2  | 1:A:418:LYS:NZ   | 0.43     | 2.84        | 13     | 1     |
| 1:A:405:THR:CG2  | 1:A:406:LEU:N    | 0.43     | 2.81        | 17     | 1     |
| 1:A:352:LEU:CD2  | 1:A:352:LEU:C    | 0.43     | 2.91        | 18     | 1     |
| 1:A:361:LEU:CD1  | 1:A:386:TYR:O    | 0.43     | 2.67        | 18     | 1     |
| 1:A:424:GLN:CD   | 1:A:424:GLN:C    | 0.43     | 2.87        | 20     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:376:TYR:CE2  | 1:A:378:THR:CG2  | 0.43     | 3.02        | 24     | 1     |
| 1:A:377:GLU:CD   | 1:A:377:GLU:C    | 0.43     | 2.87        | 1      | 3     |
| 1:A:400:LYS:O    | 1:A:402:ALA:N    | 0.43     | 2.52        | 5      | 1     |
| 1:A:421:ARG:O    | 1:A:424:GLN:CD   | 0.43     | 2.62        | 19     | 1     |
| 1:A:383:GLN:CD   | 1:A:383:GLN:C    | 0.43     | 2.87        | 25     | 1     |
| 1:A:400:LYS:CG   | 1:A:401:LYS:N    | 0.43     | 2.81        | 11     | 1     |
| 1:A:412:ALA:C    | 1:A:414:ASN:N    | 0.43     | 2.76        | 22     | 2     |
| 1:A:366:LYS:O    | 1:A:369:ASN:OD1  | 0.43     | 2.37        | 6      | 1     |
| 1:A:420:LEU:O    | 1:A:421:ARG:C    | 0.43     | 2.62        | 9      | 6     |
| 1:A:420:LEU:N    | 1:A:420:LEU:CD1  | 0.43     | 2.82        | 10     | 1     |
| 1:A:351:GLN:OE1  | 1:A:353:SER:O    | 0.43     | 2.36        | 24     | 2     |
| 1:A:360:ASN:ND2  | 1:A:360:ASN:N    | 0.43     | 2.66        | 20     | 1     |
| 1:A:358:TYR:O    | 1:A:362:ASN:OD1  | 0.43     | 2.37        | 7      | 2     |
| 1:A:359:ASP:C    | 1:A:362:ASN:OD1  | 0.43     | 2.62        | 24     | 1     |
| 1:A:368:GLU:O    | 1:A:369:ASN:CG   | 0.43     | 2.62        | 25     | 1     |
| 1:A:393:TYR:O    | 1:A:394:ALA:C    | 0.42     | 2.63        | 13     | 7     |
| 1:A:424:GLN:CD   | 1:A:424:GLN:O    | 0.42     | 2.62        | 7      | 1     |
| 1:A:378:THR:HG22 | 1:A:385:TRP:O    | 0.42     | 2.14        | 12     | 1     |
| 1:A:422:GLN:C    | 1:A:422:GLN:CD   | 0.42     | 2.87        | 15     | 3     |
| 1:A:421:ARG:O    | 1:A:424:GLN:OE1  | 0.42     | 2.37        | 16     | 2     |
| 1:A:370:LEU:O    | 1:A:371:LYS:O    | 0.42     | 2.37        | 7      | 2     |
| 1:A:346:SER:O    | 1:A:347:HIS:O    | 0.42     | 2.37        | 8      | 1     |
| 1:A:351:GLN:C    | 1:A:351:GLN:CD   | 0.42     | 2.87        | 11     | 1     |
| 1:A:397:GLU:OE1  | 1:A:397:GLU:C    | 0.42     | 2.61        | 11     | 1     |
| 1:A:405:THR:O    | 1:A:406:LEU:C    | 0.42     | 2.63        | 14     | 2     |
| 1:A:396:LYS:O    | 1:A:397:GLU:C    | 0.42     | 2.62        | 14     | 1     |
| 1:A:416:TRP:NE1  | 1:A:418:LYS:NZ   | 0.42     | 2.67        | 2      | 1     |
| 1:A:352:LEU:C    | 1:A:352:LEU:HD22 | 0.42     | 2.40        | 18     | 1     |
| 1:A:418:LYS:C    | 1:A:418:LYS:CD   | 0.42     | 2.93        | 18     | 1     |
| 1:A:353:SER:OG   | 1:A:364:TRP:CZ3  | 0.42     | 2.68        | 23     | 1     |
| 1:A:414:ASN:ND2  | 1:A:414:ASN:N    | 0.42     | 2.68        | 4      | 1     |
| 1:A:364:TRP:CE2  | 1:A:368:GLU:OE2  | 0.42     | 2.72        | 10     | 2     |
| 1:A:348:TYR:O    | 1:A:349:THR:OG1  | 0.42     | 2.37        | 9      | 1     |
| 1:A:385:TRP:NE1  | 1:A:387:VAL:HG12 | 0.42     | 2.29        | 16     | 1     |
| 1:A:351:GLN:CD   | 1:A:416:TRP:CD1  | 0.42     | 2.97        | 18     | 1     |
| 1:A:413:LYS:O    | 1:A:414:ASN:OD1  | 0.42     | 2.37        | 1      | 1     |
| 1:A:351:GLN:CD   | 1:A:351:GLN:C    | 0.42     | 2.87        | 8      | 3     |
| 1:A:359:ASP:C    | 1:A:360:ASN:HD22 | 0.42     | 2.23        | 13     | 1     |
| 1:A:349:THR:OG1  | 1:A:418:LYS:O    | 0.42     | 2.38        | 13     | 1     |
| 1:A:368:GLU:OE2  | 1:A:409:ASP:OD2  | 0.42     | 2.38        | 22     | 1     |
| 1:A:368:GLU:C    | 1:A:369:ASN:ND2  | 0.42     | 2.78        | 25     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:378:THR:CB   | 1:A:385:TRP:O    | 0.41     | 2.68        | 3      | 1     |
| 1:A:354:SER:C    | 1:A:355:SER:OG   | 0.41     | 2.62        | 4      | 2     |
| 1:A:392:VAL:HG22 | 1:A:393:TYR:N    | 0.41     | 2.29        | 6      | 2     |
| 1:A:364:TRP:CZ3  | 1:A:368:GLU:OE2  | 0.41     | 2.73        | 6      | 1     |
| 1:A:372:ASN:O    | 1:A:372:ASN:CG   | 0.41     | 2.63        | 13     | 2     |
| 1:A:354:SER:O    | 1:A:355:SER:CB   | 0.41     | 2.67        | 10     | 3     |
| 1:A:413:LYS:O    | 1:A:414:ASN:C    | 0.41     | 2.63        | 23     | 3     |
| 1:A:401:LYS:O    | 1:A:402:ALA:C    | 0.41     | 2.62        | 17     | 1     |
| 1:A:395:SER:O    | 1:A:396:LYS:C    | 0.41     | 2.62        | 20     | 1     |
| 1:A:368:GLU:CD   | 1:A:409:ASP:CG   | 0.41     | 2.89        | 21     | 1     |
| 1:A:345:SER:C    | 1:A:347:HIS:H    | 0.41     | 2.22        | 22     | 1     |
| 1:A:369:ASN:O    | 1:A:369:ASN:ND2  | 0.41     | 2.49        | 2      | 1     |
| 1:A:396:LYS:O    | 1:A:400:LYS:N    | 0.41     | 2.52        | 4      | 1     |
| 1:A:347:HIS:O    | 1:A:348:TYR:CG   | 0.41     | 2.73        | 11     | 3     |
| 1:A:403:VAL:CG1  | 1:A:404:SER:N    | 0.41     | 2.83        | 18     | 1     |
| 1:A:409:ASP:OD1  | 1:A:409:ASP:C    | 0.41     | 2.63        | 1      | 1     |
| 1:A:414:ASN:O    | 1:A:414:ASN:CG   | 0.41     | 2.62        | 1      | 1     |
| 1:A:403:VAL:HG13 | 1:A:404:SER:N    | 0.41     | 2.29        | 18     | 1     |
| 1:A:400:LYS:C    | 1:A:402:ALA:H    | 0.41     | 2.22        | 5      | 2     |
| 1:A:387:VAL:O    | 1:A:387:VAL:HG13 | 0.41     | 2.15        | 25     | 2     |
| 1:A:358:TYR:CE1  | 1:A:362:ASN:CG   | 0.41     | 2.99        | 23     | 1     |
| 1:A:399:ALA:O    | 1:A:402:ALA:HB3  | 0.41     | 2.16        | 11     | 1     |
| 1:A:387:VAL:C    | 1:A:388:LEU:HD22 | 0.41     | 2.41        | 12     | 1     |
| 1:A:373:TYR:CD1  | 1:A:373:TYR:N    | 0.41     | 2.89        | 21     | 1     |
| 1:A:366:LYS:N    | 1:A:366:LYS:CD   | 0.41     | 2.83        | 22     | 1     |
| 1:A:420:LEU:C    | 1:A:424:GLN:NE2  | 0.41     | 2.79        | 23     | 1     |
| 1:A:359:ASP:OD1  | 1:A:359:ASP:C    | 0.40     | 2.64        | 6      | 1     |
| 1:A:397:GLU:C    | 1:A:397:GLU:CD   | 0.40     | 2.89        | 11     | 1     |
| 1:A:378:THR:HG21 | 1:A:387:VAL:HG12 | 0.40     | 1.94        | 12     | 1     |
| 1:A:409:ASP:O    | 1:A:410:VAL:C    | 0.40     | 2.63        | 19     | 1     |
| 1:A:369:ASN:O    | 1:A:369:ASN:OD1  | 0.40     | 2.40        | 25     | 1     |
| 1:A:397:GLU:O    | 1:A:400:LYS:N    | 0.40     | 2.52        | 2      | 1     |
| 1:A:351:GLN:CG   | 1:A:352:LEU:N    | 0.40     | 2.83        | 5      | 1     |
| 1:A:365:ALA:O    | 1:A:368:GLU:N    | 0.40     | 2.54        | 10     | 1     |
| 1:A:413:LYS:O    | 1:A:413:LYS:CG   | 0.40     | 2.69        | 10     | 1     |
| 1:A:402:ALA:O    | 1:A:405:THR:OG1  | 0.40     | 2.36        | 22     | 1     |
| 1:A:401:LYS:C    | 1:A:403:VAL:N    | 0.40     | 2.78        | 25     | 1     |
| 1:A:413:LYS:C    | 1:A:414:ASN:OD1  | 0.40     | 2.65        | 1      | 1     |
| 1:A:375:VAL:O    | 1:A:375:VAL:CG2  | 0.40     | 2.68        | 17     | 1     |
| 1:A:414:ASN:N    | 1:A:414:ASN:HD22 | 0.40     | 2.13        | 20     | 1     |
| 1:A:383:GLN:NE2  | 1:A:384:PRO:O    | 0.40     | 2.55        | 25     | 1     |

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| Atom-1           | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|------------------|----------------|----------|-------------|--------|-------|
|                  |                |          |             | Worst  | Total |
| 1:A:390:SER:O    | 1:A:391:GLY:C  | 0.40     | 2.65        | 5      | 1     |
| 1:A:354:SER:O    | 1:A:355:SER:OG | 0.40     | 2.35        | 6      | 1     |
| 1:A:361:LEU:HD13 | 1:A:362:ASN:N  | 0.40     | 2.31        | 15     | 1     |
| 1:A:411:GLN:O    | 1:A:412:ALA:C  | 0.40     | 2.64        | 8      | 1     |
| 1:A:398:GLU:O    | 1:A:402:ALA:CB | 0.40     | 2.70        | 22     | 1     |

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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

| Mol | Chain | Analysed        | Favoured     | Allowed      | Outliers   | Percentiles |           |
|-----|-------|-----------------|--------------|--------------|------------|-------------|-----------|
| 1   | A     | 80/106 (75%)    | 60±5 (75±6%) | 15±4 (19±5%) | 5±2 (6±2%) | <b>2</b>    | <b>18</b> |
| All | All   | 2000/2650 (75%) | 1492 (75%)   | 380 (19%)    | 128 (6%)   | <b>2</b>    | <b>18</b> |

All 19 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     | 423 | VAL  | 22             |
| 1   | A     | 372 | ASN  | 21             |
| 1   | A     | 382 | GLY  | 14             |
| 1   | A     | 350 | LEU  | 13             |
| 1   | A     | 355 | SER  | 12             |
| 1   | A     | 415 | PRO  | 10             |
| 1   | A     | 397 | GLU  | 7              |
| 1   | A     | 359 | ASP  | 5              |
| 1   | A     | 371 | LYS  | 5              |
| 1   | A     | 347 | HIS  | 4              |
| 1   | A     | 421 | ARG  | 3              |
| 1   | A     | 419 | PRO  | 2              |
| 1   | A     | 391 | GLY  | 2              |
| 1   | A     | 424 | GLN  | 2              |
| 1   | A     | 400 | LYS  | 2              |
| 1   | A     | 365 | ALA  | 1              |
| 1   | A     | 409 | ASP  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 396 | LYS  | 1              |
| 1   | A     | 420 | LEU  | 1              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|-------------|----|
| 1   | A     | 70/91 (77%)     | 66±1 (95±2%) | 4±1 (5±2%) | 22          | 72 |
| All | All   | 1750/2275 (77%) | 1657 (95%)   | 93 (5%)    | 22          | 72 |

All 29 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     | 355 | SER  | 14             |
| 1   | A     | 352 | LEU  | 6              |
| 1   | A     | 372 | ASN  | 5              |
| 1   | A     | 378 | THR  | 5              |
| 1   | A     | 420 | LEU  | 5              |
| 1   | A     | 371 | LYS  | 5              |
| 1   | A     | 413 | LYS  | 4              |
| 1   | A     | 349 | THR  | 4              |
| 1   | A     | 373 | TYR  | 4              |
| 1   | A     | 401 | LYS  | 4              |
| 1   | A     | 381 | ASN  | 4              |
| 1   | A     | 360 | ASN  | 3              |
| 1   | A     | 385 | TRP  | 3              |
| 1   | A     | 396 | LYS  | 3              |
| 1   | A     | 418 | LYS  | 3              |
| 1   | A     | 351 | GLN  | 3              |
| 1   | A     | 357 | ASN  | 2              |
| 1   | A     | 400 | LYS  | 2              |
| 1   | A     | 414 | ASN  | 2              |
| 1   | A     | 377 | GLU  | 2              |
| 1   | A     | 362 | ASN  | 2              |
| 1   | A     | 369 | ASN  | 1              |
| 1   | A     | 398 | GLU  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 388 | LEU  | 1              |
| 1   | A     | 366 | LYS  | 1              |
| 1   | A     | 424 | GLN  | 1              |
| 1   | A     | 348 | TYR  | 1              |
| 1   | A     | 379 | THR  | 1              |
| 1   | A     | 387 | VAL  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 96% for the well-defined parts and 91% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1284 |
| Number of shifts mapped to atoms        | 1283 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 1    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 5    |

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

- No matching atom found in the structure. All 1 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 323 | MET  | H    | 8.453      | 0.007       | 1         |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 101      | $0.02 \pm 0.12$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 95       | $0.19 \pm 0.13$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 101      | $0.22 \pm 0.18$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 94       | $0.51 \pm 0.55$                 | None needed (imprecise)    |

### 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 96%, i.e. 1040 atoms were assigned a chemical shift out of a possible 1084. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 393/395 (99%)   | 158/159 (99%)  | 160/160 (100%)  | 75/76 (99%)     |
| Sidechain | 559/591 (95%)   | 374/382 (98%)  | 171/183 (93%)   | 14/26 (54%)     |
| Aromatic  | 88/98 (90%)     | 44/46 (96%)    | 41/47 (87%)     | 3/5 (60%)       |
| Overall   | 1040/1084 (96%) | 576/587 (98%)  | 372/390 (95%)   | 92/107 (86%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1283 atoms were assigned a chemical shift out of a possible 1415. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 497/526 (94%)   | 201/213 (94%)  | 202/212 (95%)   | 94/101 (93%)    |
| Sidechain | 679/743 (91%)   | 454/480 (95%)  | 208/229 (91%)   | 17/34 (50%)     |
| Aromatic  | 107/146 (73%)   | 56/70 (80%)    | 48/59 (81%)     | 3/17 (18%)      |
| Overall   | 1283/1415 (91%) | 711/763 (93%)  | 458/500 (92%)   | 114/152 (75%)   |

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

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

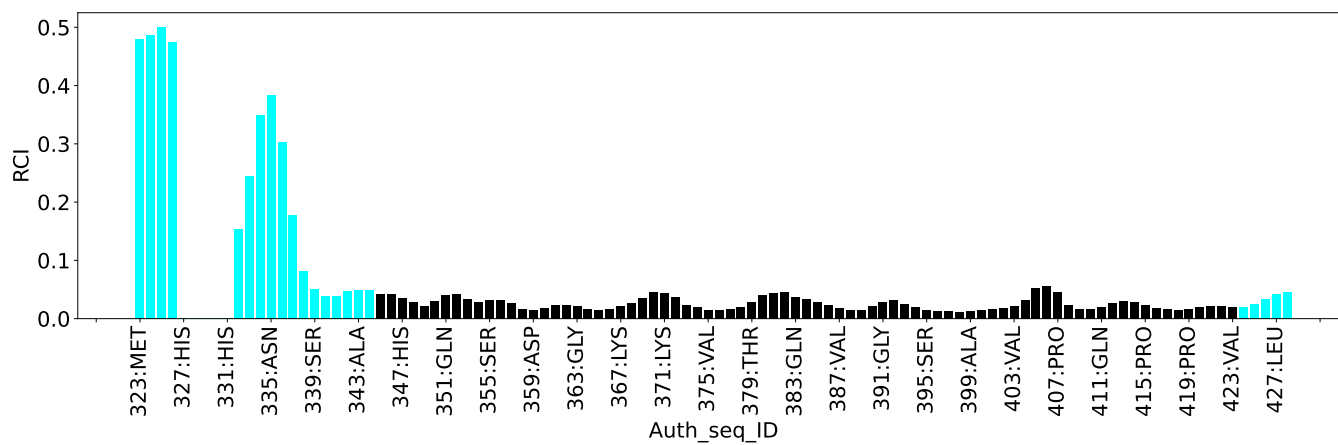
| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 405 | THR  | HG1  | 4.97       | 0.08 – 2.19         | 18.2    |
| 1       | A     | 368 | GLU  | HG3  | 0.65       | 1.20 – 3.30         | -7.6    |
| 1       | A     | 380 | ARG  | HD2  | 1.83       | 1.97 – 4.26         | -5.6    |
| 1       | A     | 368 | GLU  | HB3  | 0.84       | 0.95 – 3.05         | -5.5    |
| 1       | A     | 351 | GLN  | HB3  | 0.68       | 0.71 – 3.33         | -5.1    |

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

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

bars.

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 2804  |
| Intra-residue ( $ i-j =0$ )                              | 997   |
| Sequential ( $ i-j =1$ )                                 | 625   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 409   |
| Long range ( $ i-j \geq 5$ )                             | 773   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 162   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 28.0  |
| Number of long range restraints per residue <sup>1</sup> | 7.3   |

<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)  | 9.0                                    | 0.2     |
| 0.2-0.5 (Medium) | 6.0                                    | 0.5     |
| >0.5 (Large)     | 7.8                                    | 3.4     |

### 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)   | 1.0                                    | 2.69    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

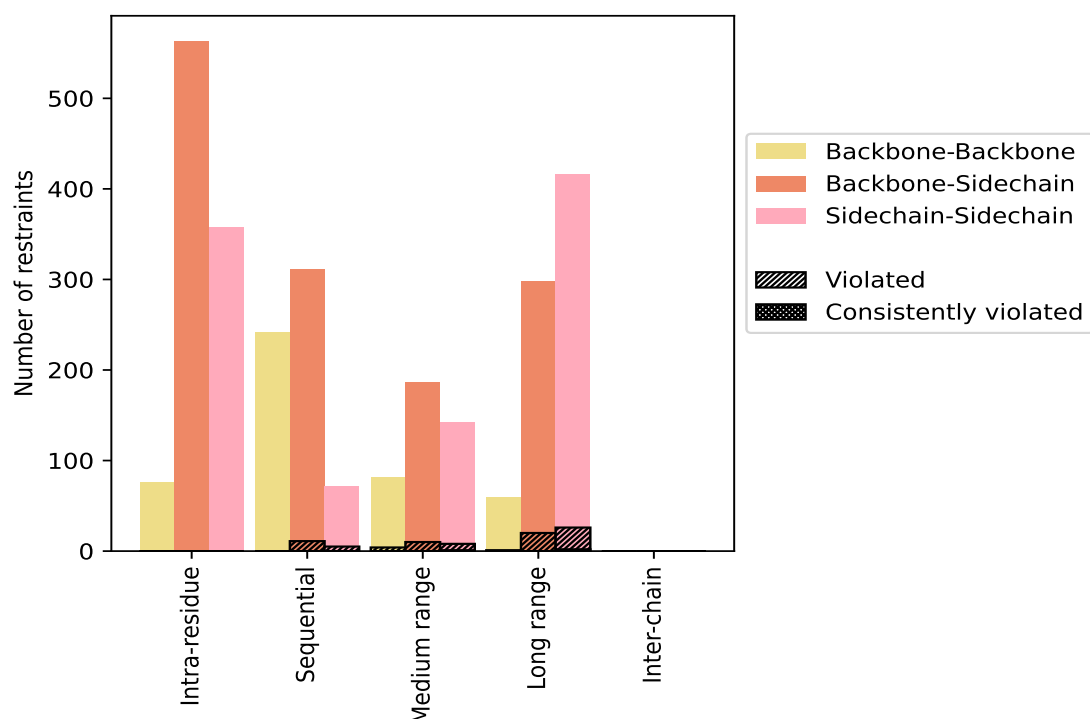
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>997</b>  | <b>35.6</b>    | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 76          | 2.7            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 563         | 20.1           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 358         | 12.8           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>625</b>  | <b>22.3</b>    | <b>16</b>             | <b>2.6</b>     | <b>0.6</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 242         | 8.6            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 311         | 11.1           | 11                    | 3.5            | 0.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 72          | 2.6            | 5                     | 6.9            | 0.2            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>409</b>  | <b>14.6</b>    | <b>22</b>             | <b>5.4</b>     | <b>0.8</b>     | <b>1</b>                           | <b>0.2</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 81          | 2.9            | 4                     | 4.9            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 186         | 6.6            | 10                    | 5.4            | 0.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 142         | 5.1            | 8                     | 5.6            | 0.3            | 1                                  | 0.7            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>773</b>  | <b>27.6</b>    | <b>47</b>             | <b>6.1</b>     | <b>1.7</b>     | <b>2</b>                           | <b>0.3</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 59          | 2.1            | 1                     | 1.7            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 298         | 10.6           | 20                    | 6.7            | 0.7            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 416         | 14.8           | 26                    | 6.2            | 0.9            | 2                                  | 0.5            | 0.1            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>2804</b> | <b>100.0</b>   | <b>85</b>             | <b>3.0</b>     | <b>3.0</b>     | <b>3</b>                           | <b>0.1</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 458         | 16.3           | 5                     | 1.1            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 1358        | 48.4           | 41                    | 3.0            | 1.5            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 988         | 35.2           | 39                    | 3.9            | 1.4            | 3                                  | 0.3            | 0.1            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 1                    | 4               | 6               | 11              | 0               | 22    | 0.5      | 1.54    | 0.43                | 0.47       |
| 2        | 1                    | 5               | 5               | 14              | 0               | 25    | 0.37     | 0.98    | 0.23                | 0.34       |
| 3        | 0                    | 5               | 6               | 14              | 0               | 25    | 0.41     | 1.7     | 0.42                | 0.23       |
| 4        | 0                    | 4               | 7               | 9               | 0               | 20    | 0.51     | 1.25    | 0.34                | 0.44       |
| 5        | 1                    | 3               | 9               | 8               | 0               | 21    | 0.38     | 1.13    | 0.26                | 0.26       |
| 6        | 0                    | 3               | 11              | 10              | 0               | 24    | 0.27     | 0.63    | 0.17                | 0.18       |
| 7        | 1                    | 5               | 7               | 12              | 0               | 25    | 0.44     | 1.53    | 0.39                | 0.24       |
| 8        | 0                    | 5               | 10              | 10              | 0               | 25    | 0.5      | 2.27    | 0.55                | 0.23       |
| 9        | 0                    | 3               | 6               | 9               | 0               | 18    | 0.47     | 1.26    | 0.36                | 0.38       |
| 10       | 0                    | 3               | 6               | 13              | 0               | 22    | 0.54     | 2.59    | 0.54                | 0.3        |

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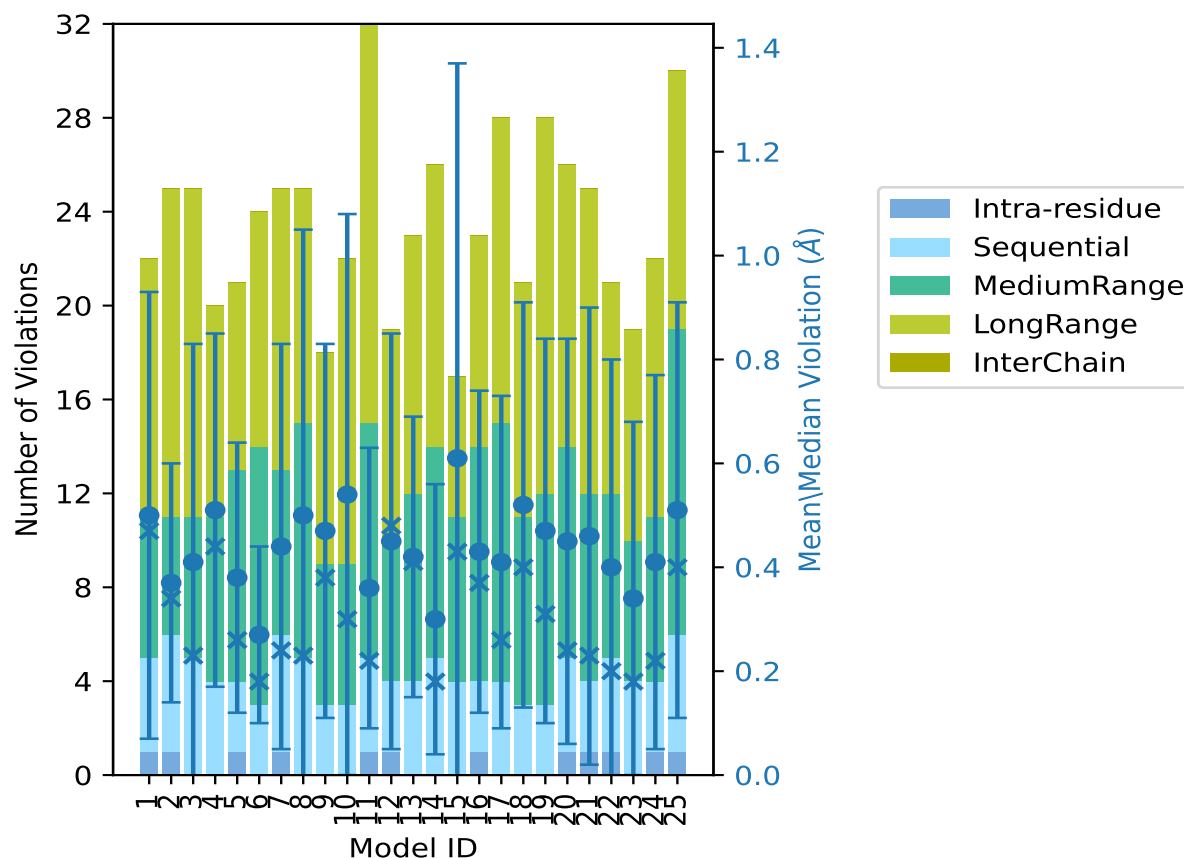
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 1                    | 4               | 10              | 17              | 0               | 32    | 0.36     | 0.96    | 0.27                | 0.22       |
| 12       | 1                    | 3               | 6               | 9               | 0               | 19    | 0.45     | 1.83    | 0.4                 | 0.48       |
| 13       | 0                    | 4               | 8               | 11              | 0               | 23    | 0.42     | 1.0     | 0.27                | 0.41       |
| 14       | 0                    | 5               | 9               | 12              | 0               | 26    | 0.3      | 1.13    | 0.26                | 0.18       |
| 15       | 0                    | 4               | 7               | 6               | 0               | 17    | 0.61     | 3.4     | 0.76                | 0.43       |
| 16       | 1                    | 3               | 10              | 9               | 0               | 23    | 0.43     | 1.13    | 0.31                | 0.37       |
| 17       | 0                    | 4               | 11              | 13              | 0               | 28    | 0.41     | 1.18    | 0.32                | 0.26       |
| 18       | 0                    | 3               | 8               | 10              | 0               | 21    | 0.52     | 1.5     | 0.39                | 0.4        |
| 19       | 0                    | 3               | 9               | 16              | 0               | 28    | 0.47     | 1.67    | 0.37                | 0.31       |
| 20       | 1                    | 4               | 9               | 12              | 0               | 26    | 0.45     | 1.61    | 0.39                | 0.24       |
| 21       | 1                    | 3               | 8               | 13              | 0               | 25    | 0.46     | 1.88    | 0.44                | 0.23       |
| 22       | 1                    | 4               | 7               | 9               | 0               | 21    | 0.4      | 1.74    | 0.4                 | 0.2        |
| 23       | 0                    | 4               | 6               | 9               | 0               | 19    | 0.34     | 1.36    | 0.34                | 0.18       |
| 24       | 1                    | 3               | 7               | 11              | 0               | 22    | 0.41     | 1.37    | 0.36                | 0.22       |
| 25       | 1                    | 5               | 13              | 11              | 0               | 30    | 0.51     | 1.59    | 0.4                 | 0.4        |

<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 [i](#)



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 [i](#)

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, 2719(IR:997, SQ:609, MR:387, LR:726, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |      |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %    |
| 0                             | 3               | 7               | 13              | 0               | 23    | 1                        | 4.0  |
| 0                             | 4               | 2               | 6               | 0               | 12    | 2                        | 8.0  |
| 0                             | 1               | 1               | 2               | 0               | 4     | 3                        | 12.0 |
| 0                             | 3               | 0               | 6               | 0               | 9     | 4                        | 16.0 |
| 0                             | 0               | 0               | 3               | 0               | 3     | 5                        | 20.0 |
| 0                             | 0               | 0               | 1               | 0               | 1     | 6                        | 24.0 |

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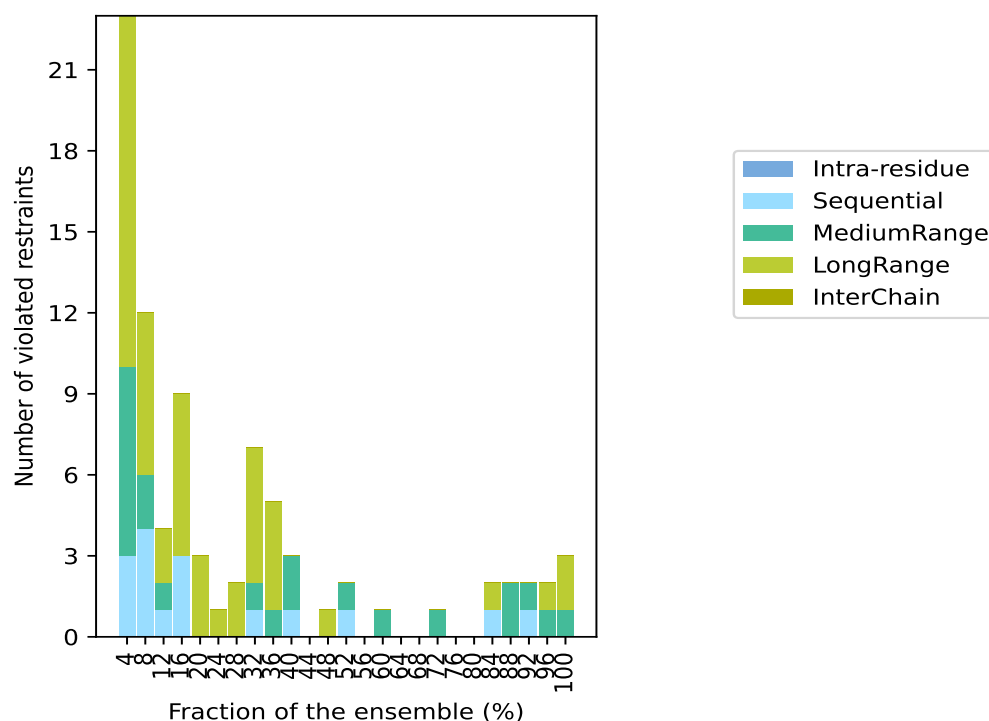
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 0                             | 0               | 0               | 2               | 0               | 2     | 7                        | 28.0  |
| 0                             | 1               | 1               | 5               | 0               | 7     | 8                        | 32.0  |
| 0                             | 0               | 1               | 4               | 0               | 5     | 9                        | 36.0  |
| 0                             | 1               | 2               | 0               | 0               | 3     | 10                       | 40.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 44.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 12                       | 48.0  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 13                       | 52.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 14                       | 56.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 15                       | 60.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 16                       | 64.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 68.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 18                       | 72.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 19                       | 76.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 20                       | 80.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 21                       | 84.0  |
| 0                             | 0               | 2               | 0               | 0               | 2     | 22                       | 88.0  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 23                       | 92.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 24                       | 96.0  |
| 0                             | 0               | 1               | 2               | 0               | 3     | 25                       | 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

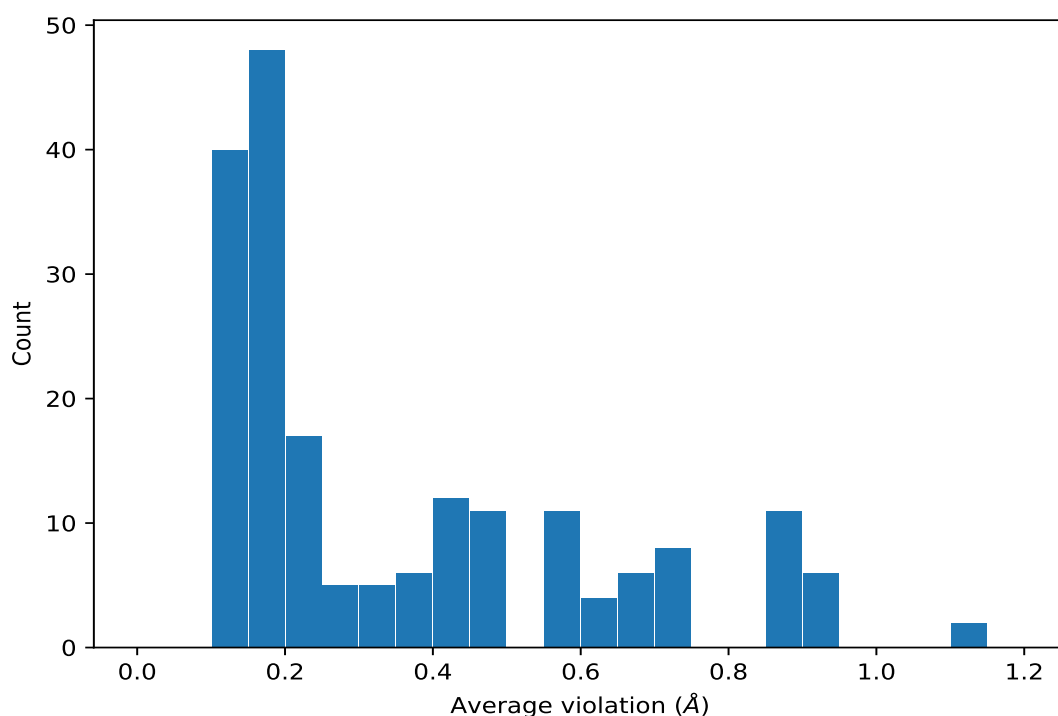
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,115)  | 1:385:A:TRP:HZ3 | 1:388:A:LEU:HG  | 25                  | 1.13     | 0.77                | 0.94       |
| (1,115)  | 1:385:A:TRP:HZ3 | 1:413:A:LYS:HD3 | 25                  | 1.13     | 0.77                | 0.94       |
| (1,195)  | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2 | 25                  | 0.65     | 0.08                | 0.67       |
| (1,195)  | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3 | 25                  | 0.65     | 0.08                | 0.67       |
| (1,196)  | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2 | 25                  | 0.65     | 0.08                | 0.67       |
| (1,196)  | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3 | 25                  | 0.65     | 0.08                | 0.67       |
| (1,77)   | 1:357:A:ASN:HB3 | 1:386:A:TYR:HD2 | 24                  | 0.89     | 0.34                | 0.98       |
| (1,77)   | 1:357:A:ASN:HB2 | 1:386:A:TYR:HD1 | 24                  | 0.89     | 0.34                | 0.98       |
| (1,77)   | 1:357:A:ASN:HB3 | 1:386:A:TYR:HE1 | 24                  | 0.89     | 0.34                | 0.98       |
| (1,77)   | 1:357:A:ASN:HB3 | 1:386:A:TYR:HD1 | 24                  | 0.89     | 0.34                | 0.98       |
| (1,77)   | 1:357:A:ASN:HB2 | 1:386:A:TYR:HE1 | 24                  | 0.89     | 0.34                | 0.98       |
| (1,177)  | 1:382:A:GLY:H   | 1:380:A:ARG:HB3 | 24                  | 0.56     | 0.15                | 0.56       |
| (1,2459) | 1:387:A:VAL:H   | 1:388:A:LEU:HB2 | 23                  | 0.21     | 0.05                | 0.22       |
| (1,2459) | 1:387:A:VAL:H   | 1:388:A:LEU:HB3 | 23                  | 0.21     | 0.05                | 0.22       |
| (1,452)  | 1:342:A:SER:HA  | 1:344:A:PRO:HD2 | 23                  | 0.18     | 0.02                | 0.17       |
| (1,452)  | 1:342:A:SER:HA  | 1:344:A:PRO:HD3 | 23                  | 0.18     | 0.02                | 0.17       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,231)  | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE1  | 22                  | 0.89     | 0.41                | 0.86       |
| (1,231)  | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 22                  | 0.89     | 0.41                | 0.86       |
| (1,231)  | 1:391:A:GLY:HA3  | 1:393:A:TYR:HD1  | 22                  | 0.89     | 0.41                | 0.86       |
| (1,236)  | 1:393:A:TYR:HE1  | 1:391:A:GLY:HA3  | 22                  | 0.89     | 0.41                | 0.86       |
| (1,236)  | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 22                  | 0.89     | 0.41                | 0.86       |
| (1,236)  | 1:393:A:TYR:HD1  | 1:391:A:GLY:HA3  | 22                  | 0.89     | 0.41                | 0.86       |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 21                  | 0.24     | 0.1                 | 0.24       |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 21                  | 0.24     | 0.1                 | 0.24       |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2  | 21                  | 0.18     | 0.05                | 0.17       |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2  | 21                  | 0.18     | 0.05                | 0.17       |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2  | 21                  | 0.18     | 0.05                | 0.17       |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2  | 21                  | 0.18     | 0.05                | 0.17       |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2  | 21                  | 0.18     | 0.05                | 0.17       |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2  | 21                  | 0.18     | 0.05                | 0.17       |
| (1,66)   | 1:352:A:LEU:HB3  | 1:415:A:PRO:HB3  | 18                  | 0.61     | 0.24                | 0.62       |
| (1,66)   | 1:352:A:LEU:HB2  | 1:415:A:PRO:HB3  | 18                  | 0.61     | 0.24                | 0.62       |
| (1,66)   | 1:352:A:LEU:HB2  | 1:350:A:LEU:HB3  | 18                  | 0.61     | 0.24                | 0.62       |
| (1,66)   | 1:352:A:LEU:HB2  | 1:350:A:LEU:HB2  | 18                  | 0.61     | 0.24                | 0.62       |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 15                  | 0.17     | 0.07                | 0.16       |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 15                  | 0.17     | 0.07                | 0.16       |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 15                  | 0.17     | 0.07                | 0.16       |
| (1,129)  | 1:367:A:LYS:H    | 1:367:A:LYS:HE3  | 13                  | 0.56     | 0.1                 | 0.59       |
| (1,129)  | 1:367:A:LYS:H    | 1:367:A:LYS:HE2  | 13                  | 0.56     | 0.1                 | 0.59       |
| (1,129)  | 1:367:A:LYS:H    | 1:366:A:LYS:HE2  | 13                  | 0.56     | 0.1                 | 0.59       |
| (1,222)  | 1:389:A:VAL:HB   | 1:387:A:VAL:HG23 | 13                  | 0.4      | 0.14                | 0.4        |
| (1,222)  | 1:389:A:VAL:HB   | 1:387:A:VAL:HG21 | 13                  | 0.4      | 0.14                | 0.4        |
| (1,222)  | 1:389:A:VAL:HB   | 1:387:A:VAL:HG22 | 13                  | 0.4      | 0.14                | 0.4        |
| (1,222)  | 1:389:A:VAL:HB   | 1:387:A:VAL:HG13 | 13                  | 0.4      | 0.14                | 0.4        |
| (1,222)  | 1:389:A:VAL:HB   | 1:392:A:VAL:HG21 | 13                  | 0.4      | 0.14                | 0.4        |
| (1,222)  | 1:389:A:VAL:HB   | 1:392:A:VAL:HG12 | 13                  | 0.4      | 0.14                | 0.4        |
| (1,222)  | 1:389:A:VAL:HB   | 1:387:A:VAL:HG11 | 13                  | 0.4      | 0.14                | 0.4        |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB2  | 12                  | 0.15     | 0.02                | 0.14       |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB3  | 12                  | 0.15     | 0.02                | 0.14       |
| (1,232)  | 1:392:A:VAL:H    | 1:393:A:TYR:HD2  | 10                  | 0.28     | 0.13                | 0.24       |
| (1,232)  | 1:392:A:VAL:H    | 1:393:A:TYR:HD1  | 10                  | 0.28     | 0.13                | 0.24       |
| (1,1976) | 1:422:A:GLN:HA   | 1:424:A:GLN:HA   | 10                  | 0.14     | 0.04                | 0.12       |
| (1,2005) | 1:424:A:GLN:HA   | 1:422:A:GLN:HA   | 10                  | 0.14     | 0.04                | 0.12       |
| (1,24)   | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD23 | 9                   | 0.94     | 0.56                | 0.69       |
| (1,24)   | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD11 | 9                   | 0.94     | 0.56                | 0.69       |
| (1,24)   | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD12 | 9                   | 0.94     | 0.56                | 0.69       |
| (1,24)   | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD13 | 9                   | 0.94     | 0.56                | 0.69       |
| (1,24)   | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD21 | 9                   | 0.94     | 0.56                | 0.69       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,24)   | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD22 | 9                   | 0.94     | 0.56                | 0.69       |
| (1,86)   | 1:358:A:TYR:HE1  | 1:362:A:ASN:HA   | 9                   | 0.57     | 0.37                | 0.42       |
| (1,86)   | 1:358:A:TYR:HE2  | 1:362:A:ASN:HA   | 9                   | 0.57     | 0.37                | 0.42       |
| (1,1305) | 1:387:A:VAL:HG11 | 1:380:A:ARG:HA   | 9                   | 0.13     | 0.02                | 0.13       |
| (1,1305) | 1:387:A:VAL:HG12 | 1:380:A:ARG:HA   | 9                   | 0.13     | 0.02                | 0.13       |
| (1,1305) | 1:387:A:VAL:HG13 | 1:380:A:ARG:HA   | 9                   | 0.13     | 0.02                | 0.13       |
| (1,1305) | 1:387:A:VAL:HG21 | 1:380:A:ARG:HA   | 9                   | 0.13     | 0.02                | 0.13       |
| (1,1305) | 1:387:A:VAL:HG22 | 1:380:A:ARG:HA   | 9                   | 0.13     | 0.02                | 0.13       |
| (1,1305) | 1:387:A:VAL:HG23 | 1:380:A:ARG:HA   | 9                   | 0.13     | 0.02                | 0.13       |
| (1,797)  | 1:364:A:TRP:HE3  | 1:385:A:TRP:HZ2  | 9                   | 0.12     | 0.01                | 0.11       |
| (1,1254) | 1:385:A:TRP:HZ2  | 1:364:A:TRP:HE3  | 9                   | 0.12     | 0.01                | 0.11       |
| (1,224)  | 1:389:A:VAL:HG23 | 1:423:A:VAL:HG21 | 8                   | 0.71     | 0.32                | 0.62       |
| (1,224)  | 1:389:A:VAL:HG11 | 1:423:A:VAL:HG11 | 8                   | 0.71     | 0.32                | 0.62       |
| (1,224)  | 1:389:A:VAL:HG12 | 1:423:A:VAL:HG12 | 8                   | 0.71     | 0.32                | 0.62       |
| (1,224)  | 1:389:A:VAL:HG12 | 1:423:A:VAL:HG21 | 8                   | 0.71     | 0.32                | 0.62       |
| (1,224)  | 1:389:A:VAL:HG13 | 1:423:A:VAL:HG12 | 8                   | 0.71     | 0.32                | 0.62       |
| (1,224)  | 1:389:A:VAL:HG12 | 1:423:A:VAL:HG22 | 8                   | 0.71     | 0.32                | 0.62       |
| (1,224)  | 1:389:A:VAL:HG21 | 1:350:A:LEU:HD23 | 8                   | 0.71     | 0.32                | 0.62       |
| (1,224)  | 1:389:A:VAL:HG13 | 1:423:A:VAL:HG11 | 8                   | 0.71     | 0.32                | 0.62       |
| (1,4)    | 1:336:A:ASN:HD21 | 1:337:A:ASN:HA   | 8                   | 0.49     | 0.15                | 0.45       |
| (1,4)    | 1:336:A:ASN:HD22 | 1:337:A:ASN:HA   | 8                   | 0.49     | 0.15                | 0.45       |
| (1,340)  | 1:423:A:VAL:HG12 | 1:427:A:LEU:HG   | 8                   | 0.47     | 0.18                | 0.49       |
| (1,340)  | 1:423:A:VAL:HG13 | 1:427:A:LEU:HG   | 8                   | 0.47     | 0.18                | 0.49       |
| (1,340)  | 1:423:A:VAL:HG11 | 1:427:A:LEU:HG   | 8                   | 0.47     | 0.18                | 0.49       |
| (1,340)  | 1:423:A:VAL:HG22 | 1:427:A:LEU:HG   | 8                   | 0.47     | 0.18                | 0.49       |
| (1,340)  | 1:423:A:VAL:HG21 | 1:427:A:LEU:HG   | 8                   | 0.47     | 0.18                | 0.49       |
| (1,1124) | 1:378:A:THR:HG21 | 1:385:A:TRP:HA   | 8                   | 0.19     | 0.06                | 0.18       |
| (1,1124) | 1:378:A:THR:HG22 | 1:385:A:TRP:HA   | 8                   | 0.19     | 0.06                | 0.18       |
| (1,1124) | 1:378:A:THR:HG23 | 1:385:A:TRP:HA   | 8                   | 0.19     | 0.06                | 0.18       |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG21 | 8                   | 0.19     | 0.06                | 0.18       |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG22 | 8                   | 0.19     | 0.06                | 0.18       |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG23 | 8                   | 0.19     | 0.06                | 0.18       |
| (1,2189) | 1:353:A:SER:H    | 1:389:A:VAL:HA   | 8                   | 0.15     | 0.02                | 0.16       |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG2  | 8                   | 0.15     | 0.04                | 0.14       |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG3  | 8                   | 0.15     | 0.04                | 0.14       |
| (1,226)  | 1:389:A:VAL:HG11 | 1:418:A:LYS:HD3  | 7                   | 0.56     | 0.3                 | 0.48       |
| (1,226)  | 1:389:A:VAL:HG12 | 1:418:A:LYS:HD3  | 7                   | 0.56     | 0.3                 | 0.48       |
| (1,226)  | 1:389:A:VAL:HG13 | 1:418:A:LYS:HD3  | 7                   | 0.56     | 0.3                 | 0.48       |
| (1,226)  | 1:389:A:VAL:HG12 | 1:418:A:LYS:HG3  | 7                   | 0.56     | 0.3                 | 0.48       |
| (1,226)  | 1:389:A:VAL:HG21 | 1:418:A:LYS:HD3  | 7                   | 0.56     | 0.3                 | 0.48       |
| (1,230)  | 1:390:A:SER:H    | 1:352:A:LEU:HG   | 7                   | 0.42     | 0.28                | 0.36       |
| (1,230)  | 1:390:A:SER:H    | 1:352:A:LEU:HB2  | 7                   | 0.42     | 0.28                | 0.36       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD1  | 6                   | 0.15     | 0.03                | 0.14       |
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD2  | 6                   | 0.15     | 0.03                | 0.14       |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD1  | 6                   | 0.15     | 0.03                | 0.14       |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD2  | 6                   | 0.15     | 0.03                | 0.14       |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD1  | 6                   | 0.15     | 0.03                | 0.14       |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD2  | 6                   | 0.15     | 0.03                | 0.14       |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD1  | 6                   | 0.15     | 0.03                | 0.14       |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD2  | 6                   | 0.15     | 0.03                | 0.14       |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD1  | 6                   | 0.15     | 0.03                | 0.14       |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD2  | 6                   | 0.15     | 0.03                | 0.14       |
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD1  | 6                   | 0.15     | 0.03                | 0.14       |
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD2  | 6                   | 0.15     | 0.03                | 0.14       |
| (1,71)   | 1:353:A:SER:H    | 1:388:A:LEU:HD12 | 5                   | 0.42     | 0.2                 | 0.43       |
| (1,71)   | 1:353:A:SER:H    | 1:388:A:LEU:HD11 | 5                   | 0.42     | 0.2                 | 0.43       |
| (1,71)   | 1:353:A:SER:H    | 1:388:A:LEU:HD13 | 5                   | 0.42     | 0.2                 | 0.43       |
| (1,153)  | 1:375:A:VAL:HB   | 1:386:A:TYR:HD2  | 5                   | 0.23     | 0.05                | 0.22       |
| (1,1224) | 1:385:A:TRP:HD1  | 1:379:A:THR:HA   | 5                   | 0.11     | 0.01                | 0.11       |
| (1,341)  | 1:423:A:VAL:HG22 | 1:420:A:LEU:HD11 | 4                   | 0.46     | 0.2                 | 0.4        |
| (1,341)  | 1:423:A:VAL:HG21 | 1:420:A:LEU:HD13 | 4                   | 0.46     | 0.2                 | 0.4        |
| (1,341)  | 1:423:A:VAL:HG22 | 1:420:A:LEU:HD12 | 4                   | 0.46     | 0.2                 | 0.4        |
| (1,341)  | 1:423:A:VAL:HG21 | 1:420:A:LEU:HD12 | 4                   | 0.46     | 0.2                 | 0.4        |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG11 | 4                   | 0.35     | 0.12                | 0.32       |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG12 | 4                   | 0.35     | 0.12                | 0.32       |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG13 | 4                   | 0.35     | 0.12                | 0.32       |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG21 | 4                   | 0.35     | 0.12                | 0.32       |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG22 | 4                   | 0.35     | 0.12                | 0.32       |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG23 | 4                   | 0.35     | 0.12                | 0.32       |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG21 | 4                   | 0.28     | 0.04                | 0.29       |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG22 | 4                   | 0.28     | 0.04                | 0.29       |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG23 | 4                   | 0.28     | 0.04                | 0.29       |
| (1,274)  | 1:403:A:VAL:HG21 | 1:415:A:PRO:HA   | 4                   | 0.19     | 0.05                | 0.18       |
| (1,274)  | 1:403:A:VAL:HG22 | 1:415:A:PRO:HA   | 4                   | 0.19     | 0.05                | 0.18       |
| (1,274)  | 1:410:A:VAL:HG13 | 1:415:A:PRO:HA   | 4                   | 0.19     | 0.05                | 0.18       |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG21 | 4                   | 0.18     | 0.01                | 0.18       |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG22 | 4                   | 0.18     | 0.01                | 0.18       |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG23 | 4                   | 0.18     | 0.01                | 0.18       |
| (1,2158) | 1:351:A:GLN:H    | 1:352:A:LEU:HB2  | 4                   | 0.14     | 0.01                | 0.15       |
| (1,2158) | 1:351:A:GLN:H    | 1:352:A:LEU:HB3  | 4                   | 0.14     | 0.01                | 0.15       |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG11 | 4                   | 0.14     | 0.03                | 0.15       |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG12 | 4                   | 0.14     | 0.03                | 0.15       |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG13 | 4                   | 0.14     | 0.03                | 0.15       |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG21 | 4                   | 0.14     | 0.03                | 0.15       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG22 | 4                   | 0.14     | 0.03                | 0.15       |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG23 | 4                   | 0.14     | 0.03                | 0.15       |
| (1,694)  | 1:356:A:SER:HB2  | 1:385:A:TRP:HZ3  | 4                   | 0.14     | 0.0                 | 0.14       |
| (1,694)  | 1:356:A:SER:HB3  | 1:385:A:TRP:HZ3  | 4                   | 0.14     | 0.0                 | 0.14       |
| (1,857)  | 1:365:A:ALA:HB1  | 1:375:A:VAL:HA   | 4                   | 0.12     | 0.01                | 0.11       |
| (1,857)  | 1:365:A:ALA:HB2  | 1:375:A:VAL:HA   | 4                   | 0.12     | 0.01                | 0.11       |
| (1,857)  | 1:365:A:ALA:HB3  | 1:375:A:VAL:HA   | 4                   | 0.12     | 0.01                | 0.11       |
| (1,37)   | 1:348:A:TYR:HB3  | 1:417:A:ALA:HB3  | 3                   | 0.32     | 0.1                 | 0.38       |
| (1,37)   | 1:348:A:TYR:HB3  | 1:417:A:ALA:HB2  | 3                   | 0.32     | 0.1                 | 0.38       |
| (1,37)   | 1:348:A:TYR:HB3  | 1:417:A:ALA:HB1  | 3                   | 0.32     | 0.1                 | 0.38       |
| (1,45)   | 1:349:A:THR:HG22 | 1:350:A:LEU:HD23 | 3                   | 0.24     | 0.07                | 0.26       |
| (1,45)   | 1:349:A:THR:HG22 | 1:423:A:VAL:HG21 | 3                   | 0.24     | 0.07                | 0.26       |
| (1,45)   | 1:349:A:THR:HG23 | 1:350:A:LEU:HD21 | 3                   | 0.24     | 0.07                | 0.26       |
| (1,41)   | 1:349:A:THR:HB   | 1:418:A:LYS:HG2  | 3                   | 0.23     | 0.1                 | 0.2        |
| (1,41)   | 1:349:A:THR:HB   | 1:420:A:LEU:HG   | 3                   | 0.23     | 0.1                 | 0.2        |
| (1,1607) | 1:405:A:THR:HG21 | 1:401:A:LYS:HG2  | 3                   | 0.15     | 0.03                | 0.16       |
| (1,1607) | 1:405:A:THR:HG21 | 1:401:A:LYS:HG3  | 3                   | 0.15     | 0.03                | 0.16       |
| (1,1607) | 1:405:A:THR:HG22 | 1:401:A:LYS:HG2  | 3                   | 0.15     | 0.03                | 0.16       |
| (1,1607) | 1:405:A:THR:HG22 | 1:401:A:LYS:HG3  | 3                   | 0.15     | 0.03                | 0.16       |
| (1,1607) | 1:405:A:THR:HG23 | 1:401:A:LYS:HG2  | 3                   | 0.15     | 0.03                | 0.16       |
| (1,1607) | 1:405:A:THR:HG23 | 1:401:A:LYS:HG3  | 3                   | 0.15     | 0.03                | 0.16       |
| (1,334)  | 1:420:A:LEU:HD11 | 1:423:A:VAL:HB   | 2                   | 0.68     | 0.19                | 0.68       |
| (1,334)  | 1:420:A:LEU:HB3  | 1:423:A:VAL:HB   | 2                   | 0.68     | 0.19                | 0.68       |
| (1,15)   | 1:420:A:LEU:HD13 | 1:423:A:VAL:HG21 | 2                   | 0.32     | 0.08                | 0.32       |
| (1,15)   | 1:420:A:LEU:HD12 | 1:423:A:VAL:HG21 | 2                   | 0.32     | 0.08                | 0.32       |
| (1,168)  | 1:378:A:THR:H    | 1:386:A:TYR:HD1  | 2                   | 0.23     | 0.0                 | 0.23       |
| (1,168)  | 1:378:A:THR:H    | 1:386:A:TYR:HD2  | 2                   | 0.23     | 0.0                 | 0.23       |
| (1,190)  | 1:385:A:TRP:HH2  | 1:358:A:TYR:HA   | 2                   | 0.22     | 0.12                | 0.22       |
| (1,624)  | 1:351:A:GLN:HG2  | 1:350:A:LEU:HB2  | 2                   | 0.2      | 0.0                 | 0.2        |
| (1,624)  | 1:351:A:GLN:HG2  | 1:350:A:LEU:HB3  | 2                   | 0.2      | 0.0                 | 0.2        |
| (1,624)  | 1:351:A:GLN:HG3  | 1:350:A:LEU:HB2  | 2                   | 0.2      | 0.0                 | 0.2        |
| (1,624)  | 1:351:A:GLN:HG3  | 1:350:A:LEU:HB3  | 2                   | 0.2      | 0.0                 | 0.2        |
| (1,225)  | 1:389:A:VAL:HG11 | 1:351:A:GLN:HG3  | 2                   | 0.19     | 0.03                | 0.19       |
| (1,225)  | 1:389:A:VAL:HG21 | 1:374:A:VAL:HB   | 2                   | 0.19     | 0.03                | 0.19       |
| (1,808)  | 1:364:A:TRP:HZ2  | 1:353:A:SER:HB2  | 2                   | 0.14     | 0.04                | 0.14       |
| (1,808)  | 1:364:A:TRP:HZ2  | 1:353:A:SER:HB3  | 2                   | 0.14     | 0.04                | 0.14       |
| (1,1593) | 1:404:A:SER:HA   | 1:403:A:VAL:HB   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,706)  | 1:358:A:TYR:HA   | 1:362:A:ASN:HB2  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,706)  | 1:358:A:TYR:HA   | 1:362:A:ASN:HB3  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1094) | 1:377:A:GLU:HG2  | 1:376:A:TYR:HE1  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1094) | 1:377:A:GLU:HG2  | 1:376:A:TYR:HE2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1094) | 1:377:A:GLU:HG3  | 1:376:A:TYR:HE1  | 2                   | 0.12     | 0.0                 | 0.12       |

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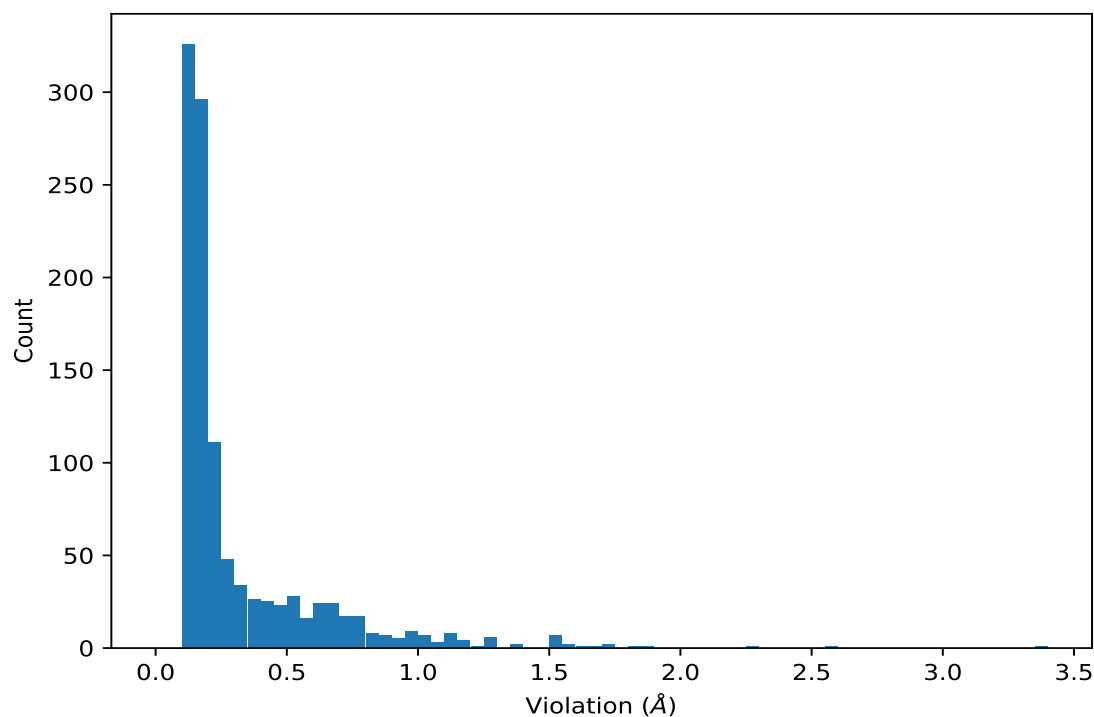
| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1094) | 1:377:A:GLU:HG3  | 1:376:A:TYR:HE2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,752)  | 1:361:A:LEU:HD11 | 1:353:A:SER:HA  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,752)  | 1:361:A:LEU:HD12 | 1:353:A:SER:HA  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,752)  | 1:361:A:LEU:HD13 | 1:353:A:SER:HA  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,752)  | 1:361:A:LEU:HD21 | 1:353:A:SER:HA  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,752)  | 1:361:A:LEU:HD22 | 1:353:A:SER:HA  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,752)  | 1:361:A:LEU:HD23 | 1:353:A:SER:HA  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1018) | 1:374:A:VAL:HB   | 1:373:A:TYR:HA  | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 15       | 3.4           |
| (1,115) | 1:385:A:TRP:HZ3  | 1:413:A:LYS:HD3  | 10       | 2.59          |
| (1,24)  | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD23 | 8        | 2.27          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:413:A:LYS:HD3  | 21       | 1.88          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 12       | 1.83          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 22       | 1.74          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 3        | 1.7           |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 19       | 1.67          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 20       | 1.61          |
| (1,236) | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 25       | 1.59          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 25       | 1.59          |
| (1,236) | 1:393:A:TYR:HE1  | 1:391:A:GLY:HA3  | 1        | 1.54          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE1  | 1        | 1.54          |
| (1,236) | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 7        | 1.53          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 7        | 1.53          |
| (1,236) | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 8        | 1.5           |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 8        | 1.5           |
| (1,24)  | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD13 | 18       | 1.5           |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 24       | 1.37          |
| (1,77)  | 1:357:A:ASN:HB2  | 1:386:A:TYR:HD1  | 23       | 1.36          |
| (1,236) | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 3        | 1.29          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 3        | 1.29          |
| (1,77)  | 1:357:A:ASN:HB3  | 1:386:A:TYR:HE1  | 24       | 1.27          |
| (1,77)  | 1:357:A:ASN:HB3  | 1:386:A:TYR:HD1  | 9        | 1.26          |
| (1,77)  | 1:357:A:ASN:HB2  | 1:386:A:TYR:HD1  | 20       | 1.26          |
| (1,77)  | 1:357:A:ASN:HB2  | 1:386:A:TYR:HD1  | 4        | 1.25          |
| (1,77)  | 1:357:A:ASN:HB3  | 1:386:A:TYR:HD1  | 8        | 1.21          |
| (1,77)  | 1:357:A:ASN:HB2  | 1:386:A:TYR:HD1  | 17       | 1.18          |
| (1,236) | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 21       | 1.17          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 21       | 1.17          |
| (1,77)  | 1:357:A:ASN:HB3  | 1:386:A:TYR:HD2  | 1        | 1.16          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 4        | 1.14          |
| (1,224) | 1:389:A:VAL:HG12 | 1:423:A:VAL:HG12 | 10       | 1.13          |
| (1,224) | 1:389:A:VAL:HG13 | 1:423:A:VAL:HG12 | 16       | 1.13          |
| (1,77)  | 1:357:A:ASN:HB3  | 1:386:A:TYR:HE1  | 5        | 1.13          |
| (1,77)  | 1:357:A:ASN:HB2  | 1:386:A:TYR:HD1  | 14       | 1.13          |
| (1,236) | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 15       | 1.11          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 15       | 1.11          |
| (1,44)  | 1:349:A:THR:HG22 | 1:418:A:LYS:HD3  | 19       | 1.11          |
| (1,236) | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 17       | 1.09          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 17       | 1.09          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,77)  | 1:357:A:ASN:HB3  | 1:386:A:TYR:HD1  | 18       | 1.08          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 23       | 1.04          |
| (1,86)  | 1:358:A:TYR:HE1  | 1:362:A:ASN:HA   | 16       | 1.03          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 9        | 1.02          |
| (1,24)  | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD11 | 4        | 1.02          |
| (1,226) | 1:389:A:VAL:HG12 | 1:418:A:LYS:HD3  | 16       | 1.0           |
| (1,224) | 1:389:A:VAL:HG12 | 1:423:A:VAL:HG22 | 18       | 1.0           |
| (1,77)  | 1:357:A:ASN:HB2  | 1:386:A:TYR:HE1  | 13       | 1.0           |
| (1,226) | 1:389:A:VAL:HG21 | 1:418:A:LYS:HD3  | 20       | 0.99          |
| (1,86)  | 1:358:A:TYR:HE1  | 1:362:A:ASN:HA   | 2        | 0.98          |
| (1,236) | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 10       | 0.97          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 10       | 0.97          |
| (1,66)  | 1:352:A:LEU:HB2  | 1:415:A:PRO:HB3  | 25       | 0.97          |
| (1,86)  | 1:358:A:TYR:HE2  | 1:362:A:ASN:HA   | 11       | 0.96          |
| (1,77)  | 1:357:A:ASN:HB2  | 1:386:A:TYR:HD1  | 7        | 0.96          |
| (1,66)  | 1:352:A:LEU:HB3  | 1:415:A:PRO:HB3  | 19       | 0.96          |
| (1,66)  | 1:352:A:LEU:HB2  | 1:415:A:PRO:HB3  | 21       | 0.96          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 18       | 0.94          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 11       | 0.93          |
| (1,236) | 1:393:A:TYR:HD1  | 1:391:A:GLY:HA3  | 22       | 0.92          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HD1  | 22       | 0.92          |
| (1,77)  | 1:357:A:ASN:HB3  | 1:386:A:TYR:HD1  | 11       | 0.9           |
| (1,236) | 1:393:A:TYR:HE1  | 1:391:A:GLY:HA3  | 9        | 0.89          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE1  | 9        | 0.89          |
| (1,230) | 1:390:A:SER:H    | 1:352:A:LEU:HG   | 4        | 0.89          |
| (1,86)  | 1:358:A:TYR:HE2  | 1:362:A:ASN:HA   | 25       | 0.89          |
| (1,334) | 1:420:A:LEU:HD11 | 1:423:A:VAL:HB   | 1        | 0.87          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 25       | 0.87          |
| (1,77)  | 1:357:A:ASN:HB3  | 1:386:A:TYR:HE1  | 12       | 0.87          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 17       | 0.84          |
| (1,340) | 1:423:A:VAL:HG13 | 1:427:A:LEU:HG   | 25       | 0.83          |
| (1,66)  | 1:352:A:LEU:HB3  | 1:415:A:PRO:HB3  | 24       | 0.83          |
| (1,236) | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 18       | 0.82          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 18       | 0.82          |
| (1,177) | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 19       | 0.82          |
| (1,66)  | 1:352:A:LEU:HB2  | 1:415:A:PRO:HB3  | 13       | 0.81          |
| (1,4)   | 1:336:A:ASN:HD21 | 1:337:A:ASN:HA   | 9        | 0.81          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 8        | 0.79          |
| (1,341) | 1:423:A:VAL:HG22 | 1:420:A:LEU:HD12 | 19       | 0.78          |
| (1,24)  | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD22 | 22       | 0.78          |
| (1,196) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 13       | 0.77          |
| (1,195) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 13       | 0.77          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,236) | 1:393:A:TYR:HE2 | 1:391:A:GLY:HA3  | 20       | 0.76          |
| (1,231) | 1:391:A:GLY:HA3 | 1:393:A:TYR:HE2  | 20       | 0.76          |
| (1,230) | 1:390:A:SER:H   | 1:352:A:LEU:HG   | 25       | 0.76          |
| (1,196) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3  | 10       | 0.76          |
| (1,195) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3  | 10       | 0.76          |
| (1,177) | 1:382:A:GLY:H   | 1:380:A:ARG:HB3  | 5        | 0.76          |
| (1,351) | 1:426:A:ASP:H   | 1:423:A:VAL:HG12 | 25       | 0.75          |
| (1,196) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2  | 14       | 0.75          |
| (1,196) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3  | 20       | 0.75          |
| (1,195) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2  | 14       | 0.75          |
| (1,195) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3  | 20       | 0.75          |
| (1,66)  | 1:352:A:LEU:HB3 | 1:415:A:PRO:HB3  | 15       | 0.75          |
| (1,177) | 1:382:A:GLY:H   | 1:380:A:ARG:HB3  | 17       | 0.74          |
| (1,196) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2  | 8        | 0.72          |
| (1,195) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2  | 8        | 0.72          |
| (1,66)  | 1:352:A:LEU:HB3 | 1:415:A:PRO:HB3  | 3        | 0.72          |
| (1,236) | 1:393:A:TYR:HE1 | 1:391:A:GLY:HA3  | 19       | 0.71          |
| (1,231) | 1:391:A:GLY:HA3 | 1:393:A:TYR:HE1  | 19       | 0.71          |
| (1,196) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2  | 3        | 0.71          |
| (1,196) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3  | 11       | 0.71          |
| (1,195) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2  | 3        | 0.71          |
| (1,195) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3  | 11       | 0.71          |
| (1,177) | 1:382:A:GLY:H   | 1:380:A:ARG:HB3  | 13       | 0.71          |
| (1,71)  | 1:353:A:SER:H   | 1:388:A:LEU:HD13 | 21       | 0.71          |
| (1,196) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2  | 12       | 0.7           |
| (1,196) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3  | 16       | 0.7           |
| (1,195) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2  | 12       | 0.7           |
| (1,195) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3  | 16       | 0.7           |
| (1,177) | 1:382:A:GLY:H   | 1:380:A:ARG:HB3  | 2        | 0.7           |
| (1,196) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2  | 5        | 0.69          |
| (1,196) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3  | 18       | 0.69          |
| (1,195) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2  | 5        | 0.69          |
| (1,195) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3  | 18       | 0.69          |
| (1,177) | 1:382:A:GLY:H   | 1:380:A:ARG:HB3  | 14       | 0.69          |
| (1,66)  | 1:352:A:LEU:HB3 | 1:415:A:PRO:HB3  | 4        | 0.69          |
| (1,24)  | 1:344:A:PRO:HG2 | 1:420:A:LEU:HD12 | 11       | 0.69          |
| (1,236) | 1:393:A:TYR:HE2 | 1:391:A:GLY:HA3  | 2        | 0.68          |
| (1,231) | 1:391:A:GLY:HA3 | 1:393:A:TYR:HE2  | 2        | 0.68          |
| (1,196) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2  | 17       | 0.68          |
| (1,195) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB2  | 17       | 0.68          |
| (1,196) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3  | 24       | 0.67          |
| (1,196) | 1:385:A:TRP:HZ3 | 1:356:A:SER:HB3  | 25       | 0.67          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,195) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB3  | 24       | 0.67          |
| (1,195) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB3  | 25       | 0.67          |
| (1,236) | 1:393:A:TYR:HE1  | 1:391:A:GLY:HA3  | 13       | 0.66          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE1  | 13       | 0.66          |
| (1,77)  | 1:357:A:ASN:HB2  | 1:386:A:TYR:HE1  | 10       | 0.66          |
| (1,77)  | 1:357:A:ASN:HB3  | 1:386:A:TYR:HE1  | 19       | 0.66          |
| (1,177) | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 24       | 0.65          |
| (1,129) | 1:367:A:LYS:H    | 1:367:A:LYS:HE3  | 1        | 0.65          |
| (1,129) | 1:367:A:LYS:H    | 1:367:A:LYS:HE3  | 21       | 0.65          |
| (1,129) | 1:367:A:LYS:H    | 1:367:A:LYS:HE3  | 25       | 0.65          |
| (1,77)  | 1:357:A:ASN:HB3  | 1:386:A:TYR:HE1  | 15       | 0.65          |
| (1,224) | 1:389:A:VAL:HG13 | 1:423:A:VAL:HG11 | 21       | 0.64          |
| (1,222) | 1:389:A:VAL:HB   | 1:387:A:VAL:HG11 | 25       | 0.64          |
| (1,196) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB3  | 4        | 0.64          |
| (1,195) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB3  | 4        | 0.64          |
| (1,129) | 1:367:A:LYS:H    | 1:367:A:LYS:HE3  | 12       | 0.64          |
| (1,129) | 1:367:A:LYS:H    | 1:367:A:LYS:HE2  | 20       | 0.64          |
| (1,66)  | 1:352:A:LEU:HB3  | 1:415:A:PRO:HB3  | 1        | 0.64          |
| (1,196) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB3  | 6        | 0.63          |
| (1,196) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 19       | 0.63          |
| (1,196) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB3  | 23       | 0.63          |
| (1,195) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB3  | 6        | 0.63          |
| (1,195) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 19       | 0.63          |
| (1,195) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB3  | 23       | 0.63          |
| (1,177) | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 10       | 0.63          |
| (1,129) | 1:367:A:LYS:H    | 1:367:A:LYS:HE3  | 22       | 0.63          |
| (1,77)  | 1:357:A:ASN:HB2  | 1:386:A:TYR:HD1  | 6        | 0.63          |
| (1,24)  | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD21 | 19       | 0.63          |
| (1,196) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 7        | 0.62          |
| (1,195) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 7        | 0.62          |
| (1,226) | 1:389:A:VAL:HG12 | 1:418:A:LYS:HG3  | 18       | 0.61          |
| (1,224) | 1:389:A:VAL:HG12 | 1:423:A:VAL:HG21 | 11       | 0.61          |
| (1,177) | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 4        | 0.61          |
| (1,177) | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 18       | 0.61          |
| (1,4)   | 1:336:A:ASN:HD22 | 1:337:A:ASN:HA   | 8        | 0.6           |
| (1,196) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 9        | 0.59          |
| (1,195) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 9        | 0.59          |
| (1,129) | 1:367:A:LYS:H    | 1:367:A:LYS:HE2  | 7        | 0.59          |
| (1,129) | 1:367:A:LYS:H    | 1:367:A:LYS:HE2  | 16       | 0.59          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 16       | 0.59          |
| (1,66)  | 1:352:A:LEU:HB2  | 1:350:A:LEU:HB2  | 20       | 0.59          |
| (1,177) | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 11       | 0.58          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,222) | 1:389:A:VAL:HB   | 1:387:A:VAL:HG22 | 14       | 0.57          |
| (1,222) | 1:389:A:VAL:HB   | 1:387:A:VAL:HG23 | 17       | 0.57          |
| (1,177) | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 1        | 0.57          |
| (1,177) | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 25       | 0.56          |
| (1,24)  | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD12 | 7        | 0.56          |
| (1,340) | 1:423:A:VAL:HG12 | 1:427:A:LEU:HG   | 7        | 0.55          |
| (1,196) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB3  | 21       | 0.55          |
| (1,195) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB3  | 21       | 0.55          |
| (1,177) | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 7        | 0.55          |
| (1,340) | 1:423:A:VAL:HG11 | 1:427:A:LEU:HG   | 15       | 0.54          |
| (1,196) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 1        | 0.54          |
| (1,196) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 2        | 0.54          |
| (1,196) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 22       | 0.54          |
| (1,195) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 1        | 0.54          |
| (1,195) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 2        | 0.54          |
| (1,195) | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 22       | 0.54          |
| (1,177) | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 8        | 0.54          |
| (1,177) | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 16       | 0.54          |
| (1,177) | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 21       | 0.54          |
| (1,340) | 1:423:A:VAL:HG12 | 1:427:A:LEU:HG   | 24       | 0.53          |
| (1,224) | 1:389:A:VAL:HG23 | 1:423:A:VAL:HG21 | 1        | 0.53          |
| (1,4)   | 1:336:A:ASN:HD22 | 1:337:A:ASN:HA   | 4        | 0.53          |
| (1,727) | 1:358:A:TYR:HA   | 1:375:A:VAL:HG11 | 13       | 0.52          |
| (1,727) | 1:358:A:TYR:HA   | 1:375:A:VAL:HG12 | 13       | 0.52          |
| (1,727) | 1:358:A:TYR:HA   | 1:375:A:VAL:HG13 | 13       | 0.52          |
| (1,727) | 1:358:A:TYR:HA   | 1:375:A:VAL:HG21 | 13       | 0.52          |
| (1,727) | 1:358:A:TYR:HA   | 1:375:A:VAL:HG22 | 13       | 0.52          |
| (1,727) | 1:358:A:TYR:HA   | 1:375:A:VAL:HG23 | 13       | 0.52          |
| (1,232) | 1:392:A:VAL:H    | 1:393:A:TYR:HD2  | 1        | 0.52          |
| (1,115) | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 13       | 0.52          |
| (1,66)  | 1:352:A:LEU:HB2  | 1:415:A:PRO:HB3  | 6        | 0.52          |
| (1,66)  | 1:352:A:LEU:HB2  | 1:350:A:LEU:HB3  | 11       | 0.52          |
| (1,71)  | 1:353:A:SER:H    | 1:388:A:LEU:HD12 | 2        | 0.51          |
| (1,24)  | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD23 | 17       | 0.51          |
| (1,177) | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 12       | 0.5           |
| (1,129) | 1:367:A:LYS:H    | 1:367:A:LYS:HE2  | 2        | 0.5           |
| (1,77)  | 1:357:A:ASN:HB2  | 1:386:A:TYR:HD1  | 25       | 0.5           |
| (1,334) | 1:420:A:LEU:HB3  | 1:423:A:VAL:HB   | 10       | 0.49          |
| (1,236) | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 5        | 0.49          |
| (1,236) | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 12       | 0.49          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 5        | 0.49          |
| (1,231) | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 12       | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,224)  | 1:389:A:VAL:HG11 | 1:423:A:VAL:HG11 | 2        | 0.49          |
| (1,177)  | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 9        | 0.49          |
| (1,115)  | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 5        | 0.49          |
| (1,236)  | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 16       | 0.48          |
| (1,232)  | 1:392:A:VAL:H    | 1:393:A:TYR:HD2  | 7        | 0.48          |
| (1,231)  | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 16       | 0.48          |
| (1,226)  | 1:389:A:VAL:HG13 | 1:418:A:LYS:HD3  | 19       | 0.48          |
| (1,66)   | 1:352:A:LEU:HB3  | 1:415:A:PRO:HB3  | 12       | 0.48          |
| (1,4)    | 1:336:A:ASN:HD21 | 1:337:A:ASN:HA   | 12       | 0.48          |
| (1,222)  | 1:389:A:VAL:HB   | 1:387:A:VAL:HG21 | 5        | 0.47          |
| (1,222)  | 1:389:A:VAL:HB   | 1:387:A:VAL:HG13 | 10       | 0.47          |
| (1,196)  | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 15       | 0.47          |
| (1,195)  | 1:385:A:TRP:HZ3  | 1:356:A:SER:HB2  | 15       | 0.47          |
| (1,129)  | 1:367:A:LYS:H    | 1:367:A:LYS:HE3  | 11       | 0.47          |
| (1,129)  | 1:367:A:LYS:H    | 1:367:A:LYS:HE2  | 5        | 0.46          |
| (1,24)   | 1:344:A:PRO:HG2  | 1:420:A:LEU:HD23 | 2        | 0.46          |
| (1,340)  | 1:423:A:VAL:HG13 | 1:427:A:LEU:HG   | 13       | 0.45          |
| (1,77)   | 1:357:A:ASN:HB3  | 1:386:A:TYR:HE1  | 21       | 0.45          |
| (1,236)  | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 4        | 0.44          |
| (1,231)  | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 4        | 0.44          |
| (1,230)  | 1:390:A:SER:H    | 1:352:A:LEU:HB2  | 11       | 0.43          |
| (1,222)  | 1:389:A:VAL:HB   | 1:387:A:VAL:HG23 | 15       | 0.43          |
| (1,129)  | 1:367:A:LYS:H    | 1:367:A:LYS:HE3  | 24       | 0.43          |
| (1,71)   | 1:353:A:SER:H    | 1:388:A:LEU:HD13 | 25       | 0.43          |
| (1,66)   | 1:352:A:LEU:HB2  | 1:415:A:PRO:HB3  | 9        | 0.43          |
| (1,86)   | 1:358:A:TYR:HE1  | 1:362:A:ASN:HA   | 20       | 0.42          |
| (1,4)    | 1:336:A:ASN:HD21 | 1:337:A:ASN:HA   | 1        | 0.42          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 20       | 0.41          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 20       | 0.41          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG11 | 17       | 0.41          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG12 | 17       | 0.41          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG13 | 17       | 0.41          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG21 | 17       | 0.41          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG22 | 17       | 0.41          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG23 | 17       | 0.41          |
| (1,341)  | 1:423:A:VAL:HG21 | 1:420:A:LEU:HD12 | 13       | 0.41          |
| (1,15)   | 1:420:A:LEU:HD12 | 1:423:A:VAL:HG21 | 13       | 0.41          |
| (1,4)    | 1:336:A:ASN:HD21 | 1:337:A:ASN:HA   | 7        | 0.41          |
| (1,341)  | 1:423:A:VAL:HG22 | 1:420:A:LEU:HD11 | 24       | 0.4           |
| (1,340)  | 1:423:A:VAL:HG12 | 1:427:A:LEU:HG   | 18       | 0.4           |
| (1,222)  | 1:389:A:VAL:HB   | 1:387:A:VAL:HG22 | 6        | 0.4           |
| (1,177)  | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 3        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,115)  | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 14       | 0.4           |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 16       | 0.39          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 16       | 0.39          |
| (1,177)  | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 23       | 0.39          |
| (1,37)   | 1:348:A:TYR:HB3  | 1:417:A:ALA:HB1  | 11       | 0.39          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 6        | 0.38          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 6        | 0.38          |
| (1,37)   | 1:348:A:TYR:HB3  | 1:417:A:ALA:HB3  | 24       | 0.38          |
| (1,4)    | 1:336:A:ASN:HD21 | 1:337:A:ASN:HA   | 11       | 0.38          |
| (1,232)  | 1:392:A:VAL:H    | 1:393:A:TYR:HD2  | 3        | 0.37          |
| (1,226)  | 1:389:A:VAL:HG13 | 1:418:A:LYS:HD3  | 17       | 0.37          |
| (1,222)  | 1:389:A:VAL:HB   | 1:392:A:VAL:HG12 | 16       | 0.37          |
| (1,177)  | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 15       | 0.37          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 25       | 0.36          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 25       | 0.36          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 25       | 0.36          |
| (1,230)  | 1:390:A:SER:H    | 1:352:A:LEU:HG   | 17       | 0.36          |
| (1,177)  | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 22       | 0.36          |
| (1,71)   | 1:353:A:SER:H    | 1:388:A:LEU:HD11 | 4        | 0.36          |
| (1,41)   | 1:349:A:THR:HB   | 1:420:A:LEU:HG   | 19       | 0.36          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 2        | 0.35          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 2        | 0.35          |
| (1,236)  | 1:393:A:TYR:HE2  | 1:391:A:GLY:HA3  | 6        | 0.35          |
| (1,231)  | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE2  | 6        | 0.35          |
| (1,222)  | 1:389:A:VAL:HB   | 1:387:A:VAL:HG21 | 8        | 0.35          |
| (1,222)  | 1:389:A:VAL:HB   | 1:387:A:VAL:HG11 | 22       | 0.35          |
| (1,190)  | 1:385:A:TRP:HH2  | 1:358:A:TYR:HA   | 2        | 0.35          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 9        | 0.34          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 9        | 0.34          |
| (1,129)  | 1:367:A:LYS:H    | 1:366:A:LYS:HE2  | 10       | 0.34          |
| (1,115)  | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 2        | 0.34          |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG21 | 17       | 0.33          |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG22 | 17       | 0.33          |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG23 | 17       | 0.33          |
| (1,77)   | 1:357:A:ASN:HB2  | 1:386:A:TYR:HD1  | 2        | 0.33          |
| (1,66)   | 1:352:A:LEU:HB3  | 1:415:A:PRO:HB3  | 23       | 0.33          |
| (1,232)  | 1:392:A:VAL:H    | 1:393:A:TYR:HD2  | 25       | 0.32          |
| (1,45)   | 1:349:A:THR:HG22 | 1:350:A:LEU:HD23 | 19       | 0.32          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 5        | 0.31          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 5        | 0.31          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 5        | 0.31          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2  | 20       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2  | 20       | 0.31          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2  | 20       | 0.31          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2  | 20       | 0.31          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2  | 20       | 0.31          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2  | 20       | 0.31          |
| (1,77)   | 1:357:A:ASN:HB3  | 1:386:A:TYR:HE1  | 3        | 0.31          |
| (1,4)    | 1:336:A:ASN:HD21 | 1:337:A:ASN:HA   | 3        | 0.31          |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG21 | 14       | 0.3           |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG22 | 14       | 0.3           |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG23 | 14       | 0.3           |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 13       | 0.3           |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 13       | 0.3           |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG21 | 19       | 0.3           |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG22 | 19       | 0.3           |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG23 | 19       | 0.3           |
| (1,1124) | 1:378:A:THR:HG21 | 1:385:A:TRP:HA   | 19       | 0.3           |
| (1,1124) | 1:378:A:THR:HG22 | 1:385:A:TRP:HA   | 19       | 0.3           |
| (1,1124) | 1:378:A:THR:HG23 | 1:385:A:TRP:HA   | 19       | 0.3           |
| (1,153)  | 1:375:A:VAL:HB   | 1:386:A:TYR:HD2  | 3        | 0.3           |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 1        | 0.29          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 1        | 0.29          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 21       | 0.29          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 21       | 0.29          |
| (1,226)  | 1:389:A:VAL:HG11 | 1:418:A:LYS:HD3  | 6        | 0.29          |
| (1,153)  | 1:375:A:VAL:HB   | 1:386:A:TYR:HD2  | 19       | 0.28          |
| (1,86)   | 1:358:A:TYR:HE1  | 1:362:A:ASN:HA   | 4        | 0.28          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 16       | 0.27          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 16       | 0.27          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 17       | 0.27          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 17       | 0.27          |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG21 | 2        | 0.27          |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG22 | 2        | 0.27          |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG23 | 2        | 0.27          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 23       | 0.27          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 23       | 0.27          |
| (1,222)  | 1:389:A:VAL:HB   | 1:392:A:VAL:HG21 | 11       | 0.27          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 18       | 0.26          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 18       | 0.26          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 19       | 0.26          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 19       | 0.26          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG21 | 5        | 0.26          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG22 | 5        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG23 | 5        | 0.26          |
| (1,1124) | 1:378:A:THR:HG21 | 1:385:A:TRP:HA   | 5        | 0.26          |
| (1,1124) | 1:378:A:THR:HG22 | 1:385:A:TRP:HA   | 5        | 0.26          |
| (1,1124) | 1:378:A:THR:HG23 | 1:385:A:TRP:HA   | 5        | 0.26          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2  | 10       | 0.26          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2  | 10       | 0.26          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2  | 10       | 0.26          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2  | 10       | 0.26          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2  | 10       | 0.26          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2  | 10       | 0.26          |
| (1,274)  | 1:403:A:VAL:HG21 | 1:415:A:PRO:HA   | 5        | 0.26          |
| (1,115)  | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 7        | 0.26          |
| (1,45)   | 1:349:A:THR:HG22 | 1:423:A:VAL:HG21 | 11       | 0.26          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 1        | 0.25          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 1        | 0.25          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 5        | 0.25          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 5        | 0.25          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 8        | 0.25          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 8        | 0.25          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 22       | 0.25          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 22       | 0.25          |
| (1,232)  | 1:392:A:VAL:H    | 1:393:A:TYR:HD2  | 8        | 0.25          |
| (1,222)  | 1:389:A:VAL:HB   | 1:387:A:VAL:HG23 | 3        | 0.25          |
| (1,77)   | 1:357:A:ASN:HB2  | 1:386:A:TYR:HD1  | 16       | 0.25          |
| (1,66)   | 1:352:A:LEU:HB2  | 1:415:A:PRO:HB3  | 14       | 0.25          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 24       | 0.24          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 24       | 0.24          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 7        | 0.24          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 7        | 0.24          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG11 | 14       | 0.24          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG12 | 14       | 0.24          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG13 | 14       | 0.24          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG21 | 14       | 0.24          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG22 | 14       | 0.24          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG23 | 14       | 0.24          |
| (1,675)  | 1:354:A:SER:HA   | 1:387:A:VAL:HB   | 10       | 0.24          |
| (1,341)  | 1:423:A:VAL:HG21 | 1:420:A:LEU:HD13 | 17       | 0.24          |
| (1,340)  | 1:423:A:VAL:HG22 | 1:427:A:LEU:HG   | 20       | 0.24          |
| (1,86)   | 1:358:A:TYR:HE1  | 1:362:A:ASN:HA   | 18       | 0.24          |
| (1,66)   | 1:352:A:LEU:HB3  | 1:415:A:PRO:HB3  | 16       | 0.24          |
| (1,15)   | 1:420:A:LEU:HD13 | 1:423:A:VAL:HG21 | 17       | 0.24          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 6        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 6        | 0.23          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG21 | 3        | 0.23          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG22 | 3        | 0.23          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG23 | 3        | 0.23          |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG2  | 20       | 0.23          |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG3  | 20       | 0.23          |
| (1,1124) | 1:378:A:THR:HG21 | 1:385:A:TRP:HA   | 3        | 0.23          |
| (1,1124) | 1:378:A:THR:HG22 | 1:385:A:TRP:HA   | 3        | 0.23          |
| (1,1124) | 1:378:A:THR:HG23 | 1:385:A:TRP:HA   | 3        | 0.23          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2  | 14       | 0.23          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2  | 14       | 0.23          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2  | 14       | 0.23          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2  | 14       | 0.23          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2  | 14       | 0.23          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2  | 14       | 0.23          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 8        | 0.23          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 8        | 0.23          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 19       | 0.23          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 19       | 0.23          |
| (1,408)  | 1:334:A:SER:HA   | 1:332:A:HIS:HA   | 14       | 0.23          |
| (1,340)  | 1:423:A:VAL:HG21 | 1:427:A:LEU:HG   | 21       | 0.23          |
| (1,331)  | 1:419:A:PRO:HD2  | 1:416:A:TRP:HH2  | 6        | 0.23          |
| (1,168)  | 1:378:A:THR:H    | 1:386:A:TYR:HD2  | 7        | 0.23          |
| (1,168)  | 1:378:A:THR:H    | 1:386:A:TYR:HD1  | 11       | 0.23          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 4        | 0.22          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 4        | 0.22          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 7        | 0.22          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 7        | 0.22          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 11       | 0.22          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 11       | 0.22          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 13       | 0.22          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 13       | 0.22          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 23       | 0.22          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 23       | 0.22          |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG21 | 13       | 0.22          |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG22 | 13       | 0.22          |
| (1,2384) | 1:377:A:GLU:H    | 1:378:A:THR:HG23 | 13       | 0.22          |
| (1,1195) | 1:384:A:PRO:HB2  | 1:379:A:THR:HB   | 20       | 0.22          |
| (1,1195) | 1:384:A:PRO:HB3  | 1:379:A:THR:HB   | 20       | 0.22          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2  | 4        | 0.22          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2  | 4        | 0.22          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2  | 4        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2  | 4        | 0.22          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2  | 4        | 0.22          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2  | 4        | 0.22          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2  | 11       | 0.22          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2  | 11       | 0.22          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2  | 11       | 0.22          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2  | 11       | 0.22          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2  | 11       | 0.22          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2  | 11       | 0.22          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2  | 25       | 0.22          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2  | 25       | 0.22          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2  | 25       | 0.22          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2  | 25       | 0.22          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2  | 25       | 0.22          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2  | 25       | 0.22          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG11 | 9        | 0.22          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG12 | 9        | 0.22          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG13 | 9        | 0.22          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG21 | 9        | 0.22          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG22 | 9        | 0.22          |
| (1,727)  | 1:358:A:TYR:HA   | 1:375:A:VAL:HG23 | 9        | 0.22          |
| (1,274)  | 1:403:A:VAL:HG21 | 1:415:A:PRO:HA   | 25       | 0.22          |
| (1,232)  | 1:392:A:VAL:H    | 1:393:A:TYR:HD2  | 10       | 0.22          |
| (1,225)  | 1:389:A:VAL:HG11 | 1:351:A:GLN:HG3  | 25       | 0.22          |
| (1,153)  | 1:375:A:VAL:HB   | 1:386:A:TYR:HD2  | 10       | 0.22          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 25       | 0.21          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 25       | 0.21          |
| (1,2338) | 1:371:A:LYS:H    | 1:373:A:TYR:HE1  | 16       | 0.21          |
| (1,2338) | 1:371:A:LYS:H    | 1:373:A:TYR:HE2  | 16       | 0.21          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 4        | 0.21          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 4        | 0.21          |
| (1,66)   | 1:352:A:LEU:HB3  | 1:415:A:PRO:HB3  | 7        | 0.21          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 2        | 0.2           |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 2        | 0.2           |
| (1,2005) | 1:424:A:GLN:HA   | 1:422:A:GLN:HA   | 25       | 0.2           |
| (1,1976) | 1:422:A:GLN:HA   | 1:424:A:GLN:HA   | 25       | 0.2           |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG2  | 21       | 0.2           |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG3  | 21       | 0.2           |
| (1,624)  | 1:351:A:GLN:HG2  | 1:350:A:LEU:HB2  | 8        | 0.2           |
| (1,624)  | 1:351:A:GLN:HG2  | 1:350:A:LEU:HB3  | 8        | 0.2           |
| (1,624)  | 1:351:A:GLN:HG3  | 1:350:A:LEU:HB2  | 8        | 0.2           |
| (1,624)  | 1:351:A:GLN:HG3  | 1:350:A:LEU:HB3  | 8        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,624)  | 1:351:A:GLN:HG2  | 1:350:A:LEU:HB2  | 10       | 0.2           |
| (1,624)  | 1:351:A:GLN:HG2  | 1:350:A:LEU:HB3  | 10       | 0.2           |
| (1,624)  | 1:351:A:GLN:HG3  | 1:350:A:LEU:HB2  | 10       | 0.2           |
| (1,624)  | 1:351:A:GLN:HG3  | 1:350:A:LEU:HB3  | 10       | 0.2           |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 14       | 0.2           |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 14       | 0.2           |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 22       | 0.2           |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 22       | 0.2           |
| (1,230)  | 1:390:A:SER:H    | 1:352:A:LEU:HG   | 10       | 0.2           |
| (1,41)   | 1:349:A:THR:HB   | 1:418:A:LYS:HG2  | 24       | 0.2           |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 9        | 0.19          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 9        | 0.19          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 15       | 0.19          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 15       | 0.19          |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG21 | 2        | 0.19          |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG22 | 2        | 0.19          |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG23 | 2        | 0.19          |
| (1,2189) | 1:353:A:SER:H    | 1:389:A:VAL:HA   | 5        | 0.19          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 11       | 0.19          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 11       | 0.19          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 11       | 0.19          |
| (1,2005) | 1:424:A:GLN:HA   | 1:422:A:GLN:HA   | 20       | 0.19          |
| (1,1976) | 1:422:A:GLN:HA   | 1:424:A:GLN:HA   | 20       | 0.19          |
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD1  | 6        | 0.19          |
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD2  | 6        | 0.19          |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD1  | 6        | 0.19          |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD2  | 6        | 0.19          |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD1  | 6        | 0.19          |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD2  | 6        | 0.19          |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD1  | 6        | 0.19          |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD2  | 6        | 0.19          |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD1  | 6        | 0.19          |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD2  | 6        | 0.19          |
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD1  | 6        | 0.19          |
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD2  | 6        | 0.19          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB2  | 13       | 0.19          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB3  | 13       | 0.19          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 13       | 0.19          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 13       | 0.19          |
| (1,232)  | 1:392:A:VAL:H    | 1:393:A:TYR:HD2  | 18       | 0.19          |
| (1,88)   | 1:358:A:TYR:HE1  | 1:375:A:VAL:HB   | 20       | 0.19          |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG21 | 14       | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG22 | 14       | 0.18          |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG23 | 14       | 0.18          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG11 | 20       | 0.18          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG12 | 20       | 0.18          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG13 | 20       | 0.18          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG21 | 20       | 0.18          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG22 | 20       | 0.18          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG23 | 20       | 0.18          |
| (1,2005) | 1:424:A:GLN:HA   | 1:422:A:GLN:HA   | 23       | 0.18          |
| (1,1976) | 1:422:A:GLN:HA   | 1:424:A:GLN:HA   | 23       | 0.18          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 5        | 0.18          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 5        | 0.18          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG21 | 14       | 0.18          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG22 | 14       | 0.18          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG23 | 14       | 0.18          |
| (1,1124) | 1:378:A:THR:HG21 | 1:385:A:TRP:HA   | 14       | 0.18          |
| (1,1124) | 1:378:A:THR:HG22 | 1:385:A:TRP:HA   | 14       | 0.18          |
| (1,1124) | 1:378:A:THR:HG23 | 1:385:A:TRP:HA   | 14       | 0.18          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2  | 17       | 0.18          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2  | 17       | 0.18          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2  | 17       | 0.18          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2  | 17       | 0.18          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2  | 17       | 0.18          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2  | 17       | 0.18          |
| (1,808)  | 1:364:A:TRP:HZ2  | 1:353:A:SER:HB2  | 18       | 0.18          |
| (1,808)  | 1:364:A:TRP:HZ2  | 1:353:A:SER:HB3  | 18       | 0.18          |
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD1  | 16       | 0.18          |
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD2  | 16       | 0.18          |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD1  | 16       | 0.18          |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD2  | 16       | 0.18          |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD1  | 16       | 0.18          |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD2  | 16       | 0.18          |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD1  | 16       | 0.18          |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD2  | 16       | 0.18          |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD1  | 16       | 0.18          |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD2  | 16       | 0.18          |
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD1  | 16       | 0.18          |
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD2  | 16       | 0.18          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 3        | 0.18          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 3        | 0.18          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 7        | 0.18          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 7        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 9        | 0.18          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 9        | 0.18          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 15       | 0.18          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 15       | 0.18          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 18       | 0.18          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 18       | 0.18          |
| (1,226)  | 1:389:A:VAL:HG12 | 1:418:A:LYS:HD3  | 23       | 0.18          |
| (1,153)  | 1:375:A:VAL:HB   | 1:386:A:TYR:HD2  | 6        | 0.18          |
| (1,37)   | 1:348:A:TYR:HB3  | 1:417:A:ALA:HB2  | 10       | 0.18          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 14       | 0.17          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 14       | 0.17          |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG21 | 17       | 0.17          |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG22 | 17       | 0.17          |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG23 | 17       | 0.17          |
| (1,2189) | 1:353:A:SER:H    | 1:389:A:VAL:HA   | 19       | 0.17          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 7        | 0.17          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 7        | 0.17          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 7        | 0.17          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 8        | 0.17          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 8        | 0.17          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 8        | 0.17          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 18       | 0.17          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 18       | 0.17          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 18       | 0.17          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 22       | 0.17          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 22       | 0.17          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 22       | 0.17          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 11       | 0.17          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 11       | 0.17          |
| (1,1607) | 1:405:A:THR:HG21 | 1:401:A:LYS:HG2  | 17       | 0.17          |
| (1,1607) | 1:405:A:THR:HG21 | 1:401:A:LYS:HG3  | 17       | 0.17          |
| (1,1607) | 1:405:A:THR:HG22 | 1:401:A:LYS:HG2  | 17       | 0.17          |
| (1,1607) | 1:405:A:THR:HG22 | 1:401:A:LYS:HG3  | 17       | 0.17          |
| (1,1607) | 1:405:A:THR:HG23 | 1:401:A:LYS:HG2  | 17       | 0.17          |
| (1,1607) | 1:405:A:THR:HG23 | 1:401:A:LYS:HG3  | 17       | 0.17          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG21 | 2        | 0.17          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG22 | 2        | 0.17          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG23 | 2        | 0.17          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG21 | 17       | 0.17          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG22 | 17       | 0.17          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG23 | 17       | 0.17          |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG2  | 6        | 0.17          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG3 | 6        | 0.17          |
| (1,1124) | 1:378:A:THR:HG21 | 1:385:A:TRP:HA  | 2        | 0.17          |
| (1,1124) | 1:378:A:THR:HG22 | 1:385:A:TRP:HA  | 2        | 0.17          |
| (1,1124) | 1:378:A:THR:HG23 | 1:385:A:TRP:HA  | 2        | 0.17          |
| (1,1124) | 1:378:A:THR:HG21 | 1:385:A:TRP:HA  | 17       | 0.17          |
| (1,1124) | 1:378:A:THR:HG22 | 1:385:A:TRP:HA  | 17       | 0.17          |
| (1,1124) | 1:378:A:THR:HG23 | 1:385:A:TRP:HA  | 17       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2 | 3        | 0.17          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2 | 3        | 0.17          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2 | 3        | 0.17          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2 | 3        | 0.17          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2 | 3        | 0.17          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2 | 3        | 0.17          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2 | 15       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2 | 15       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2 | 15       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2 | 15       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2 | 15       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2 | 15       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2 | 16       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2 | 16       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2 | 16       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2 | 16       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2 | 16       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2 | 16       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2 | 21       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2 | 21       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2 | 21       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2 | 21       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2 | 21       | 0.17          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2 | 21       | 0.17          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB2 | 21       | 0.17          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB3 | 21       | 0.17          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB2 | 23       | 0.17          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB3 | 23       | 0.17          |
| (1,631)  | 1:352:A:LEU:HG   | 1:351:A:GLN:HA  | 11       | 0.17          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2 | 16       | 0.17          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3 | 16       | 0.17          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2 | 24       | 0.17          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3 | 24       | 0.17          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2 | 25       | 0.17          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3 | 25       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,232)  | 1:392:A:VAL:H    | 1:393:A:TYR:HD1  | 15       | 0.17          |
| (1,153)  | 1:375:A:VAL:HB   | 1:386:A:TYR:HD2  | 22       | 0.17          |
| (1,33)   | 1:347:A:HIS:HD2  | 1:344:A:PRO:HB2  | 17       | 0.17          |
| (1,2755) | 1:422:A:GLN:H    | 1:423:A:VAL:HB   | 2        | 0.16          |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG21 | 13       | 0.16          |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG22 | 13       | 0.16          |
| (1,2397) | 1:379:A:THR:H    | 1:378:A:THR:HG23 | 13       | 0.16          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG11 | 25       | 0.16          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG12 | 25       | 0.16          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG13 | 25       | 0.16          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG21 | 25       | 0.16          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG22 | 25       | 0.16          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG23 | 25       | 0.16          |
| (1,2189) | 1:353:A:SER:H    | 1:389:A:VAL:HA   | 20       | 0.16          |
| (1,2189) | 1:353:A:SER:H    | 1:389:A:VAL:HA   | 24       | 0.16          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 14       | 0.16          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 14       | 0.16          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 14       | 0.16          |
| (1,1951) | 1:420:A:LEU:HD11 | 1:421:A:ARG:HB2  | 7        | 0.16          |
| (1,1951) | 1:420:A:LEU:HD11 | 1:421:A:ARG:HB3  | 7        | 0.16          |
| (1,1951) | 1:420:A:LEU:HD12 | 1:421:A:ARG:HB2  | 7        | 0.16          |
| (1,1951) | 1:420:A:LEU:HD12 | 1:421:A:ARG:HB3  | 7        | 0.16          |
| (1,1951) | 1:420:A:LEU:HD13 | 1:421:A:ARG:HB2  | 7        | 0.16          |
| (1,1951) | 1:420:A:LEU:HD13 | 1:421:A:ARG:HB3  | 7        | 0.16          |
| (1,1951) | 1:420:A:LEU:HD21 | 1:421:A:ARG:HB2  | 7        | 0.16          |
| (1,1951) | 1:420:A:LEU:HD21 | 1:421:A:ARG:HB3  | 7        | 0.16          |
| (1,1951) | 1:420:A:LEU:HD22 | 1:421:A:ARG:HB2  | 7        | 0.16          |
| (1,1951) | 1:420:A:LEU:HD22 | 1:421:A:ARG:HB3  | 7        | 0.16          |
| (1,1951) | 1:420:A:LEU:HD23 | 1:421:A:ARG:HB2  | 7        | 0.16          |
| (1,1951) | 1:420:A:LEU:HD23 | 1:421:A:ARG:HB3  | 7        | 0.16          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 12       | 0.16          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 12       | 0.16          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 18       | 0.16          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 18       | 0.16          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 24       | 0.16          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 24       | 0.16          |
| (1,1607) | 1:405:A:THR:HG21 | 1:401:A:LYS:HG2  | 12       | 0.16          |
| (1,1607) | 1:405:A:THR:HG21 | 1:401:A:LYS:HG3  | 12       | 0.16          |
| (1,1607) | 1:405:A:THR:HG22 | 1:401:A:LYS:HG2  | 12       | 0.16          |
| (1,1607) | 1:405:A:THR:HG22 | 1:401:A:LYS:HG3  | 12       | 0.16          |
| (1,1607) | 1:405:A:THR:HG23 | 1:401:A:LYS:HG2  | 12       | 0.16          |
| (1,1607) | 1:405:A:THR:HG23 | 1:401:A:LYS:HG3  | 12       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1305) | 1:387:A:VAL:HG11 | 1:380:A:ARG:HA   | 19       | 0.16          |
| (1,1305) | 1:387:A:VAL:HG12 | 1:380:A:ARG:HA   | 19       | 0.16          |
| (1,1305) | 1:387:A:VAL:HG13 | 1:380:A:ARG:HA   | 19       | 0.16          |
| (1,1305) | 1:387:A:VAL:HG21 | 1:380:A:ARG:HA   | 19       | 0.16          |
| (1,1305) | 1:387:A:VAL:HG22 | 1:380:A:ARG:HA   | 19       | 0.16          |
| (1,1305) | 1:387:A:VAL:HG23 | 1:380:A:ARG:HA   | 19       | 0.16          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2  | 12       | 0.16          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2  | 12       | 0.16          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2  | 12       | 0.16          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2  | 12       | 0.16          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2  | 12       | 0.16          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2  | 12       | 0.16          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2  | 23       | 0.16          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2  | 23       | 0.16          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2  | 23       | 0.16          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2  | 23       | 0.16          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2  | 23       | 0.16          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2  | 23       | 0.16          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB2  | 7        | 0.16          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB3  | 7        | 0.16          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 1        | 0.16          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 1        | 0.16          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 6        | 0.16          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 6        | 0.16          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 11       | 0.16          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 11       | 0.16          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 12       | 0.16          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 12       | 0.16          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 21       | 0.16          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 21       | 0.16          |
| (1,230)  | 1:390:A:SER:H    | 1:352:A:LEU:HG   | 8        | 0.16          |
| (1,225)  | 1:389:A:VAL:HG21 | 1:374:A:VAL:HB   | 11       | 0.16          |
| (1,224)  | 1:389:A:VAL:HG21 | 1:350:A:LEU:HD23 | 20       | 0.16          |
| (1,115)  | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 1        | 0.16          |
| (1,69)   | 1:353:A:SER:HB2  | 1:361:A:LEU:HD13 | 7        | 0.16          |
| (1,2189) | 1:353:A:SER:H    | 1:389:A:VAL:HA   | 3        | 0.15          |
| (1,2158) | 1:351:A:GLN:H    | 1:352:A:LEU:HB2  | 5        | 0.15          |
| (1,2158) | 1:351:A:GLN:H    | 1:352:A:LEU:HB3  | 5        | 0.15          |
| (1,2158) | 1:351:A:GLN:H    | 1:352:A:LEU:HB2  | 14       | 0.15          |
| (1,2158) | 1:351:A:GLN:H    | 1:352:A:LEU:HB3  | 14       | 0.15          |
| (1,2158) | 1:351:A:GLN:H    | 1:352:A:LEU:HB2  | 23       | 0.15          |
| (1,2158) | 1:351:A:GLN:H    | 1:352:A:LEU:HB3  | 23       | 0.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB  | 9        | 0.15          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB  | 9        | 0.15          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB  | 9        | 0.15          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB  | 24       | 0.15          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB  | 24       | 0.15          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB  | 24       | 0.15          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2 | 14       | 0.15          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3 | 14       | 0.15          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2 | 19       | 0.15          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3 | 19       | 0.15          |
| (1,1305) | 1:387:A:VAL:HG11 | 1:380:A:ARG:HA  | 25       | 0.15          |
| (1,1305) | 1:387:A:VAL:HG12 | 1:380:A:ARG:HA  | 25       | 0.15          |
| (1,1305) | 1:387:A:VAL:HG13 | 1:380:A:ARG:HA  | 25       | 0.15          |
| (1,1305) | 1:387:A:VAL:HG21 | 1:380:A:ARG:HA  | 25       | 0.15          |
| (1,1305) | 1:387:A:VAL:HG22 | 1:380:A:ARG:HA  | 25       | 0.15          |
| (1,1305) | 1:387:A:VAL:HG23 | 1:380:A:ARG:HA  | 25       | 0.15          |
| (1,1254) | 1:385:A:TRP:HZ2  | 1:364:A:TRP:HE3 | 7        | 0.15          |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG2 | 3        | 0.15          |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG3 | 3        | 0.15          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2 | 2        | 0.15          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2 | 2        | 0.15          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2 | 2        | 0.15          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2 | 2        | 0.15          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2 | 2        | 0.15          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2 | 2        | 0.15          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2 | 8        | 0.15          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2 | 8        | 0.15          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2 | 8        | 0.15          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2 | 8        | 0.15          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2 | 8        | 0.15          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2 | 8        | 0.15          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2 | 13       | 0.15          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2 | 13       | 0.15          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2 | 13       | 0.15          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2 | 13       | 0.15          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2 | 13       | 0.15          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2 | 13       | 0.15          |
| (1,797)  | 1:364:A:TRP:HE3  | 1:385:A:TRP:HZ2 | 7        | 0.15          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB2 | 24       | 0.15          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB3 | 24       | 0.15          |
| (1,694)  | 1:356:A:SER:HB2  | 1:385:A:TRP:HZ3 | 10       | 0.15          |
| (1,694)  | 1:356:A:SER:HB3  | 1:385:A:TRP:HZ3 | 10       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 5        | 0.15          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 5        | 0.15          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 10       | 0.15          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 10       | 0.15          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 17       | 0.15          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 17       | 0.15          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD2  | 23       | 0.15          |
| (1,452)  | 1:342:A:SER:HA   | 1:344:A:PRO:HD3  | 23       | 0.15          |
| (1,274)  | 1:403:A:VAL:HG22 | 1:415:A:PRO:HA   | 2        | 0.15          |
| (1,115)  | 1:385:A:TRP:HZ3  | 1:388:A:LEU:HG   | 6        | 0.15          |
| (1,86)   | 1:358:A:TYR:HE1  | 1:362:A:ASN:HA   | 24       | 0.15          |
| (1,45)   | 1:349:A:THR:HG23 | 1:350:A:LEU:HD21 | 4        | 0.15          |
| (1,2727) | 1:418:A:LYS:H    | 1:389:A:VAL:HG11 | 1        | 0.14          |
| (1,2727) | 1:418:A:LYS:H    | 1:389:A:VAL:HG12 | 1        | 0.14          |
| (1,2727) | 1:418:A:LYS:H    | 1:389:A:VAL:HG13 | 1        | 0.14          |
| (1,2727) | 1:418:A:LYS:H    | 1:389:A:VAL:HG21 | 1        | 0.14          |
| (1,2727) | 1:418:A:LYS:H    | 1:389:A:VAL:HG22 | 1        | 0.14          |
| (1,2727) | 1:418:A:LYS:H    | 1:389:A:VAL:HG23 | 1        | 0.14          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 3        | 0.14          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 3        | 0.14          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 12       | 0.14          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 12       | 0.14          |
| (1,2189) | 1:353:A:SER:H    | 1:389:A:VAL:HA   | 14       | 0.14          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 19       | 0.14          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 19       | 0.14          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 19       | 0.14          |
| (1,1305) | 1:387:A:VAL:HG11 | 1:380:A:ARG:HA   | 1        | 0.14          |
| (1,1305) | 1:387:A:VAL:HG12 | 1:380:A:ARG:HA   | 1        | 0.14          |
| (1,1305) | 1:387:A:VAL:HG13 | 1:380:A:ARG:HA   | 1        | 0.14          |
| (1,1305) | 1:387:A:VAL:HG21 | 1:380:A:ARG:HA   | 1        | 0.14          |
| (1,1305) | 1:387:A:VAL:HG22 | 1:380:A:ARG:HA   | 1        | 0.14          |
| (1,1305) | 1:387:A:VAL:HG23 | 1:380:A:ARG:HA   | 1        | 0.14          |
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD1  | 3        | 0.14          |
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD2  | 3        | 0.14          |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD1  | 3        | 0.14          |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD2  | 3        | 0.14          |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD1  | 3        | 0.14          |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD2  | 3        | 0.14          |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD1  | 3        | 0.14          |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD2  | 3        | 0.14          |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD1  | 3        | 0.14          |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD2  | 3        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD1  | 3        | 0.14          |
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD2  | 3        | 0.14          |
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD1  | 11       | 0.14          |
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD2  | 11       | 0.14          |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD1  | 11       | 0.14          |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD2  | 11       | 0.14          |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD1  | 11       | 0.14          |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD2  | 11       | 0.14          |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD1  | 11       | 0.14          |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD2  | 11       | 0.14          |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD1  | 11       | 0.14          |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD2  | 11       | 0.14          |
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD1  | 11       | 0.14          |
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD2  | 11       | 0.14          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB2  | 12       | 0.14          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB3  | 12       | 0.14          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB2  | 17       | 0.14          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB3  | 17       | 0.14          |
| (1,706)  | 1:358:A:TYR:HA   | 1:362:A:ASN:HB2  | 25       | 0.14          |
| (1,706)  | 1:358:A:TYR:HA   | 1:362:A:ASN:HB3  | 25       | 0.14          |
| (1,694)  | 1:356:A:SER:HB2  | 1:385:A:TRP:HZ3  | 3        | 0.14          |
| (1,694)  | 1:356:A:SER:HB3  | 1:385:A:TRP:HZ3  | 3        | 0.14          |
| (1,694)  | 1:356:A:SER:HB2  | 1:385:A:TRP:HZ3  | 13       | 0.14          |
| (1,694)  | 1:356:A:SER:HB3  | 1:385:A:TRP:HZ3  | 13       | 0.14          |
| (1,694)  | 1:356:A:SER:HB2  | 1:385:A:TRP:HZ3  | 14       | 0.14          |
| (1,694)  | 1:356:A:SER:HB3  | 1:385:A:TRP:HZ3  | 14       | 0.14          |
| (1,177)  | 1:382:A:GLY:H    | 1:380:A:ARG:HB3  | 6        | 0.14          |
| (1,105)  | 1:361:A:LEU:HD13 | 1:354:A:SER:HA   | 10       | 0.14          |
| (1,86)   | 1:358:A:TYR:HE1  | 1:362:A:ASN:HA   | 8        | 0.14          |
| (1,2496) | 1:392:A:VAL:H    | 1:390:A:SER:HA   | 14       | 0.13          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG11 | 17       | 0.13          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG12 | 17       | 0.13          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG13 | 17       | 0.13          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG21 | 17       | 0.13          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG22 | 17       | 0.13          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG23 | 17       | 0.13          |
| (1,2189) | 1:353:A:SER:H    | 1:389:A:VAL:HA   | 12       | 0.13          |
| (1,2158) | 1:351:A:GLN:H    | 1:352:A:LEU:HB2  | 16       | 0.13          |
| (1,2158) | 1:351:A:GLN:H    | 1:352:A:LEU:HB3  | 16       | 0.13          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 6        | 0.13          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 6        | 0.13          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 6        | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2 | 3        | 0.13          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3 | 3        | 0.13          |
| (1,1593) | 1:404:A:SER:HA   | 1:403:A:VAL:HB  | 4        | 0.13          |
| (1,1305) | 1:387:A:VAL:HG11 | 1:380:A:ARG:HA  | 4        | 0.13          |
| (1,1305) | 1:387:A:VAL:HG12 | 1:380:A:ARG:HA  | 4        | 0.13          |
| (1,1305) | 1:387:A:VAL:HG13 | 1:380:A:ARG:HA  | 4        | 0.13          |
| (1,1305) | 1:387:A:VAL:HG21 | 1:380:A:ARG:HA  | 4        | 0.13          |
| (1,1305) | 1:387:A:VAL:HG22 | 1:380:A:ARG:HA  | 4        | 0.13          |
| (1,1305) | 1:387:A:VAL:HG23 | 1:380:A:ARG:HA  | 4        | 0.13          |
| (1,1305) | 1:387:A:VAL:HG11 | 1:380:A:ARG:HA  | 11       | 0.13          |
| (1,1305) | 1:387:A:VAL:HG12 | 1:380:A:ARG:HA  | 11       | 0.13          |
| (1,1305) | 1:387:A:VAL:HG13 | 1:380:A:ARG:HA  | 11       | 0.13          |
| (1,1305) | 1:387:A:VAL:HG21 | 1:380:A:ARG:HA  | 11       | 0.13          |
| (1,1305) | 1:387:A:VAL:HG22 | 1:380:A:ARG:HA  | 11       | 0.13          |
| (1,1305) | 1:387:A:VAL:HG23 | 1:380:A:ARG:HA  | 11       | 0.13          |
| (1,1254) | 1:385:A:TRP:HZ2  | 1:364:A:TRP:HE3 | 11       | 0.13          |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG2 | 25       | 0.13          |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG3 | 25       | 0.13          |
| (1,1097) | 1:377:A:GLU:HG2  | 1:386:A:TYR:HA  | 24       | 0.13          |
| (1,1097) | 1:377:A:GLU:HG3  | 1:386:A:TYR:HA  | 24       | 0.13          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2 | 5        | 0.13          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2 | 5        | 0.13          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2 | 5        | 0.13          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2 | 5        | 0.13          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2 | 5        | 0.13          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2 | 5        | 0.13          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2 | 6        | 0.13          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2 | 6        | 0.13          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2 | 6        | 0.13          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2 | 6        | 0.13          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2 | 6        | 0.13          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2 | 6        | 0.13          |
| (1,857)  | 1:365:A:ALA:HB1  | 1:375:A:VAL:HA  | 24       | 0.13          |
| (1,857)  | 1:365:A:ALA:HB2  | 1:375:A:VAL:HA  | 24       | 0.13          |
| (1,857)  | 1:365:A:ALA:HB3  | 1:375:A:VAL:HA  | 24       | 0.13          |
| (1,797)  | 1:364:A:TRP:HE3  | 1:385:A:TRP:HZ2 | 11       | 0.13          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB2 | 3        | 0.13          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB3 | 3        | 0.13          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB2 | 9        | 0.13          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB3 | 9        | 0.13          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB2 | 18       | 0.13          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB3 | 18       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB2  | 19       | 0.13          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB3  | 19       | 0.13          |
| (1,274)  | 1:410:A:VAL:HG13 | 1:415:A:PRO:HA   | 23       | 0.13          |
| (1,232)  | 1:392:A:VAL:H    | 1:393:A:TYR:HD2  | 20       | 0.13          |
| (1,232)  | 1:392:A:VAL:H    | 1:393:A:TYR:HD2  | 21       | 0.13          |
| (1,230)  | 1:390:A:SER:H    | 1:352:A:LEU:HG   | 18       | 0.13          |
| (1,41)   | 1:349:A:THR:HB   | 1:420:A:LEU:HG   | 17       | 0.13          |
| (1,40)   | 1:349:A:THR:HA   | 1:392:A:VAL:HG13 | 8        | 0.13          |
| (1,2573) | 1:400:A:LYS:H    | 1:396:A:LYS:HD2  | 6        | 0.12          |
| (1,2573) | 1:400:A:LYS:H    | 1:396:A:LYS:HD3  | 6        | 0.12          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 20       | 0.12          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 20       | 0.12          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB2  | 22       | 0.12          |
| (1,2459) | 1:387:A:VAL:H    | 1:388:A:LEU:HB3  | 22       | 0.12          |
| (1,2189) | 1:353:A:SER:H    | 1:389:A:VAL:HA   | 22       | 0.12          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 17       | 0.12          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 17       | 0.12          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 17       | 0.12          |
| (1,2005) | 1:424:A:GLN:HA   | 1:422:A:GLN:HA   | 8        | 0.12          |
| (1,2005) | 1:424:A:GLN:HA   | 1:422:A:GLN:HA   | 19       | 0.12          |
| (1,2005) | 1:424:A:GLN:HA   | 1:422:A:GLN:HA   | 21       | 0.12          |
| (1,1976) | 1:422:A:GLN:HA   | 1:424:A:GLN:HA   | 8        | 0.12          |
| (1,1976) | 1:422:A:GLN:HA   | 1:424:A:GLN:HA   | 19       | 0.12          |
| (1,1976) | 1:422:A:GLN:HA   | 1:424:A:GLN:HA   | 21       | 0.12          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 15       | 0.12          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 15       | 0.12          |
| (1,1593) | 1:404:A:SER:HA   | 1:403:A:VAL:HB   | 25       | 0.12          |
| (1,1305) | 1:387:A:VAL:HG11 | 1:380:A:ARG:HA   | 8        | 0.12          |
| (1,1305) | 1:387:A:VAL:HG12 | 1:380:A:ARG:HA   | 8        | 0.12          |
| (1,1305) | 1:387:A:VAL:HG13 | 1:380:A:ARG:HA   | 8        | 0.12          |
| (1,1305) | 1:387:A:VAL:HG21 | 1:380:A:ARG:HA   | 8        | 0.12          |
| (1,1305) | 1:387:A:VAL:HG22 | 1:380:A:ARG:HA   | 8        | 0.12          |
| (1,1305) | 1:387:A:VAL:HG23 | 1:380:A:ARG:HA   | 8        | 0.12          |
| (1,1254) | 1:385:A:TRP:HZ2  | 1:364:A:TRP:HE3  | 19       | 0.12          |
| (1,1254) | 1:385:A:TRP:HZ2  | 1:364:A:TRP:HE3  | 22       | 0.12          |
| (1,1224) | 1:385:A:TRP:HD1  | 1:379:A:THR:HA   | 8        | 0.12          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG21 | 13       | 0.12          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG22 | 13       | 0.12          |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG23 | 13       | 0.12          |
| (1,1161) | 1:380:A:ARG:HB2  | 1:385:A:TRP:HE3  | 12       | 0.12          |
| (1,1161) | 1:380:A:ARG:HB3  | 1:385:A:TRP:HE3  | 12       | 0.12          |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG2  | 24       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG3  | 24       | 0.12          |
| (1,1124) | 1:378:A:THR:HG21 | 1:385:A:TRP:HA   | 13       | 0.12          |
| (1,1124) | 1:378:A:THR:HG22 | 1:385:A:TRP:HA   | 13       | 0.12          |
| (1,1124) | 1:378:A:THR:HG23 | 1:385:A:TRP:HA   | 13       | 0.12          |
| (1,1094) | 1:377:A:GLU:HG2  | 1:376:A:TYR:HE1  | 22       | 0.12          |
| (1,1094) | 1:377:A:GLU:HG2  | 1:376:A:TYR:HE2  | 22       | 0.12          |
| (1,1094) | 1:377:A:GLU:HG3  | 1:376:A:TYR:HE1  | 22       | 0.12          |
| (1,1094) | 1:377:A:GLU:HG3  | 1:376:A:TYR:HE2  | 22       | 0.12          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2  | 9        | 0.12          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2  | 9        | 0.12          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2  | 9        | 0.12          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2  | 9        | 0.12          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2  | 9        | 0.12          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2  | 9        | 0.12          |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2  | 24       | 0.12          |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2  | 24       | 0.12          |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2  | 24       | 0.12          |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2  | 24       | 0.12          |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2  | 24       | 0.12          |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2  | 24       | 0.12          |
| (1,797)  | 1:364:A:TRP:HE3  | 1:385:A:TRP:HZ2  | 19       | 0.12          |
| (1,797)  | 1:364:A:TRP:HE3  | 1:385:A:TRP:HZ2  | 22       | 0.12          |
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD1  | 2        | 0.12          |
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD2  | 2        | 0.12          |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD1  | 2        | 0.12          |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD2  | 2        | 0.12          |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD1  | 2        | 0.12          |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD2  | 2        | 0.12          |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD1  | 2        | 0.12          |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD2  | 2        | 0.12          |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD1  | 2        | 0.12          |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD2  | 2        | 0.12          |
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD1  | 2        | 0.12          |
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD2  | 2        | 0.12          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB2  | 1        | 0.12          |
| (1,742)  | 1:361:A:LEU:HG   | 1:355:A:SER:HB3  | 1        | 0.12          |
| (1,236)  | 1:393:A:TYR:HE1  | 1:391:A:GLY:HA3  | 11       | 0.12          |
| (1,231)  | 1:391:A:GLY:HA3  | 1:393:A:TYR:HE1  | 11       | 0.12          |
| (1,55)   | 1:350:A:LEU:HD11 | 1:403:A:VAL:HA   | 2        | 0.12          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG11 | 8        | 0.11          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG12 | 8        | 0.11          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG13 | 8        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG21 | 8        | 0.11          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG22 | 8        | 0.11          |
| (1,2294) | 1:366:A:LYS:H    | 1:375:A:VAL:HG23 | 8        | 0.11          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 20       | 0.11          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 20       | 0.11          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 20       | 0.11          |
| (1,2021) | 1:425:A:ALA:HB1  | 1:423:A:VAL:HB   | 21       | 0.11          |
| (1,2021) | 1:425:A:ALA:HB2  | 1:423:A:VAL:HB   | 21       | 0.11          |
| (1,2021) | 1:425:A:ALA:HB3  | 1:423:A:VAL:HB   | 21       | 0.11          |
| (1,2005) | 1:424:A:GLN:HA   | 1:422:A:GLN:HA   | 5        | 0.11          |
| (1,2005) | 1:424:A:GLN:HA   | 1:422:A:GLN:HA   | 6        | 0.11          |
| (1,2005) | 1:424:A:GLN:HA   | 1:422:A:GLN:HA   | 14       | 0.11          |
| (1,1976) | 1:422:A:GLN:HA   | 1:424:A:GLN:HA   | 5        | 0.11          |
| (1,1976) | 1:422:A:GLN:HA   | 1:424:A:GLN:HA   | 6        | 0.11          |
| (1,1976) | 1:422:A:GLN:HA   | 1:424:A:GLN:HA   | 14       | 0.11          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG2  | 17       | 0.11          |
| (1,1754) | 1:414:A:ASN:HA   | 1:413:A:LYS:HG3  | 17       | 0.11          |
| (1,1607) | 1:405:A:THR:HG21 | 1:401:A:LYS:HG2  | 4        | 0.11          |
| (1,1607) | 1:405:A:THR:HG21 | 1:401:A:LYS:HG3  | 4        | 0.11          |
| (1,1607) | 1:405:A:THR:HG22 | 1:401:A:LYS:HG2  | 4        | 0.11          |
| (1,1607) | 1:405:A:THR:HG22 | 1:401:A:LYS:HG3  | 4        | 0.11          |
| (1,1607) | 1:405:A:THR:HG23 | 1:401:A:LYS:HG2  | 4        | 0.11          |
| (1,1607) | 1:405:A:THR:HG23 | 1:401:A:LYS:HG3  | 4        | 0.11          |
| (1,1305) | 1:387:A:VAL:HG11 | 1:380:A:ARG:HA   | 7        | 0.11          |
| (1,1305) | 1:387:A:VAL:HG12 | 1:380:A:ARG:HA   | 7        | 0.11          |
| (1,1305) | 1:387:A:VAL:HG13 | 1:380:A:ARG:HA   | 7        | 0.11          |
| (1,1305) | 1:387:A:VAL:HG21 | 1:380:A:ARG:HA   | 7        | 0.11          |
| (1,1305) | 1:387:A:VAL:HG22 | 1:380:A:ARG:HA   | 7        | 0.11          |
| (1,1305) | 1:387:A:VAL:HG23 | 1:380:A:ARG:HA   | 7        | 0.11          |
| (1,1305) | 1:387:A:VAL:HG11 | 1:380:A:ARG:HA   | 21       | 0.11          |
| (1,1305) | 1:387:A:VAL:HG12 | 1:380:A:ARG:HA   | 21       | 0.11          |
| (1,1305) | 1:387:A:VAL:HG13 | 1:380:A:ARG:HA   | 21       | 0.11          |
| (1,1305) | 1:387:A:VAL:HG21 | 1:380:A:ARG:HA   | 21       | 0.11          |
| (1,1305) | 1:387:A:VAL:HG22 | 1:380:A:ARG:HA   | 21       | 0.11          |
| (1,1305) | 1:387:A:VAL:HG23 | 1:380:A:ARG:HA   | 21       | 0.11          |
| (1,1254) | 1:385:A:TRP:HZ2  | 1:364:A:TRP:HE3  | 1        | 0.11          |
| (1,1254) | 1:385:A:TRP:HZ2  | 1:364:A:TRP:HE3  | 6        | 0.11          |
| (1,1254) | 1:385:A:TRP:HZ2  | 1:364:A:TRP:HE3  | 20       | 0.11          |
| (1,1224) | 1:385:A:TRP:HD1  | 1:379:A:THR:HA   | 11       | 0.11          |
| (1,1224) | 1:385:A:TRP:HD1  | 1:379:A:THR:HA   | 18       | 0.11          |
| (1,1224) | 1:385:A:TRP:HD1  | 1:379:A:THR:HA   | 22       | 0.11          |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG2  | 15       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG3  | 15       | 0.11          |
| (1,1094) | 1:377:A:GLU:HG2  | 1:376:A:TYR:HE1  | 23       | 0.11          |
| (1,1094) | 1:377:A:GLU:HG2  | 1:376:A:TYR:HE2  | 23       | 0.11          |
| (1,1094) | 1:377:A:GLU:HG3  | 1:376:A:TYR:HE1  | 23       | 0.11          |
| (1,1094) | 1:377:A:GLU:HG3  | 1:376:A:TYR:HE2  | 23       | 0.11          |
| (1,1018) | 1:374:A:VAL:HB   | 1:373:A:TYR:HA   | 8        | 0.11          |
| (1,857)  | 1:365:A:ALA:HB1  | 1:375:A:VAL:HA   | 15       | 0.11          |
| (1,857)  | 1:365:A:ALA:HB2  | 1:375:A:VAL:HA   | 15       | 0.11          |
| (1,857)  | 1:365:A:ALA:HB3  | 1:375:A:VAL:HA   | 15       | 0.11          |
| (1,857)  | 1:365:A:ALA:HB1  | 1:375:A:VAL:HA   | 21       | 0.11          |
| (1,857)  | 1:365:A:ALA:HB2  | 1:375:A:VAL:HA   | 21       | 0.11          |
| (1,857)  | 1:365:A:ALA:HB3  | 1:375:A:VAL:HA   | 21       | 0.11          |
| (1,857)  | 1:365:A:ALA:HB1  | 1:375:A:VAL:HA   | 23       | 0.11          |
| (1,857)  | 1:365:A:ALA:HB2  | 1:375:A:VAL:HA   | 23       | 0.11          |
| (1,857)  | 1:365:A:ALA:HB3  | 1:375:A:VAL:HA   | 23       | 0.11          |
| (1,797)  | 1:364:A:TRP:HE3  | 1:385:A:TRP:HZ2  | 1        | 0.11          |
| (1,797)  | 1:364:A:TRP:HE3  | 1:385:A:TRP:HZ2  | 6        | 0.11          |
| (1,797)  | 1:364:A:TRP:HE3  | 1:385:A:TRP:HZ2  | 20       | 0.11          |
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD1  | 12       | 0.11          |
| (1,762)  | 1:361:A:LEU:HD11 | 1:376:A:TYR:HD2  | 12       | 0.11          |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD1  | 12       | 0.11          |
| (1,762)  | 1:361:A:LEU:HD12 | 1:376:A:TYR:HD2  | 12       | 0.11          |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD1  | 12       | 0.11          |
| (1,762)  | 1:361:A:LEU:HD13 | 1:376:A:TYR:HD2  | 12       | 0.11          |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD1  | 12       | 0.11          |
| (1,762)  | 1:361:A:LEU:HD21 | 1:376:A:TYR:HD2  | 12       | 0.11          |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD1  | 12       | 0.11          |
| (1,762)  | 1:361:A:LEU:HD22 | 1:376:A:TYR:HD2  | 12       | 0.11          |
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD1  | 12       | 0.11          |
| (1,762)  | 1:361:A:LEU:HD23 | 1:376:A:TYR:HD2  | 12       | 0.11          |
| (1,752)  | 1:361:A:LEU:HD11 | 1:353:A:SER:HA   | 9        | 0.11          |
| (1,752)  | 1:361:A:LEU:HD12 | 1:353:A:SER:HA   | 9        | 0.11          |
| (1,752)  | 1:361:A:LEU:HD13 | 1:353:A:SER:HA   | 9        | 0.11          |
| (1,752)  | 1:361:A:LEU:HD21 | 1:353:A:SER:HA   | 9        | 0.11          |
| (1,752)  | 1:361:A:LEU:HD22 | 1:353:A:SER:HA   | 9        | 0.11          |
| (1,752)  | 1:361:A:LEU:HD23 | 1:353:A:SER:HA   | 9        | 0.11          |
| (1,656)  | 1:353:A:SER:HA   | 1:387:A:VAL:HG11 | 16       | 0.11          |
| (1,656)  | 1:353:A:SER:HA   | 1:387:A:VAL:HG12 | 16       | 0.11          |
| (1,656)  | 1:353:A:SER:HA   | 1:387:A:VAL:HG13 | 16       | 0.11          |
| (1,656)  | 1:353:A:SER:HA   | 1:387:A:VAL:HG21 | 16       | 0.11          |
| (1,656)  | 1:353:A:SER:HA   | 1:387:A:VAL:HG22 | 16       | 0.11          |
| (1,656)  | 1:353:A:SER:HA   | 1:387:A:VAL:HG23 | 16       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,222)  | 1:389:A:VAL:HB   | 1:387:A:VAL:HG23 | 23       | 0.11          |
| (1,71)   | 1:353:A:SER:H    | 1:388:A:LEU:HD12 | 13       | 0.11          |
| (1,2005) | 1:424:A:GLN:HA   | 1:422:A:GLN:HA   | 16       | 0.1           |
| (1,1976) | 1:422:A:GLN:HA   | 1:424:A:GLN:HA   | 16       | 0.1           |
| (1,1847) | 1:417:A:ALA:HB1  | 1:350:A:LEU:HG   | 10       | 0.1           |
| (1,1847) | 1:417:A:ALA:HB2  | 1:350:A:LEU:HG   | 10       | 0.1           |
| (1,1847) | 1:417:A:ALA:HB3  | 1:350:A:LEU:HG   | 10       | 0.1           |
| (1,1305) | 1:387:A:VAL:HG11 | 1:380:A:ARG:HA   | 9        | 0.1           |
| (1,1305) | 1:387:A:VAL:HG12 | 1:380:A:ARG:HA   | 9        | 0.1           |
| (1,1305) | 1:387:A:VAL:HG13 | 1:380:A:ARG:HA   | 9        | 0.1           |
| (1,1305) | 1:387:A:VAL:HG21 | 1:380:A:ARG:HA   | 9        | 0.1           |
| (1,1305) | 1:387:A:VAL:HG22 | 1:380:A:ARG:HA   | 9        | 0.1           |
| (1,1305) | 1:387:A:VAL:HG23 | 1:380:A:ARG:HA   | 9        | 0.1           |
| (1,1254) | 1:385:A:TRP:HZ2  | 1:364:A:TRP:HE3  | 3        | 0.1           |
| (1,1254) | 1:385:A:TRP:HZ2  | 1:364:A:TRP:HE3  | 14       | 0.1           |
| (1,1224) | 1:385:A:TRP:HD1  | 1:379:A:THR:HA   | 7        | 0.1           |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG21 | 21       | 0.1           |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG22 | 21       | 0.1           |
| (1,1210) | 1:385:A:TRP:HA   | 1:378:A:THR:HG23 | 21       | 0.1           |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG2  | 22       | 0.1           |
| (1,1140) | 1:379:A:THR:HB   | 1:380:A:ARG:HG3  | 22       | 0.1           |
| (1,1124) | 1:378:A:THR:HG21 | 1:385:A:TRP:HA   | 21       | 0.1           |
| (1,1124) | 1:378:A:THR:HG22 | 1:385:A:TRP:HA   | 21       | 0.1           |
| (1,1124) | 1:378:A:THR:HG23 | 1:385:A:TRP:HA   | 21       | 0.1           |
| (1,1018) | 1:374:A:VAL:HB   | 1:373:A:TYR:HA   | 25       | 0.1           |
| (1,950)  | 1:370:A:LEU:HD11 | 1:385:A:TRP:HH2  | 1        | 0.1           |
| (1,950)  | 1:370:A:LEU:HD12 | 1:385:A:TRP:HH2  | 1        | 0.1           |
| (1,950)  | 1:370:A:LEU:HD13 | 1:385:A:TRP:HH2  | 1        | 0.1           |
| (1,950)  | 1:370:A:LEU:HD21 | 1:385:A:TRP:HH2  | 1        | 0.1           |
| (1,950)  | 1:370:A:LEU:HD22 | 1:385:A:TRP:HH2  | 1        | 0.1           |
| (1,950)  | 1:370:A:LEU:HD23 | 1:385:A:TRP:HH2  | 1        | 0.1           |
| (1,808)  | 1:364:A:TRP:HZ2  | 1:353:A:SER:HB2  | 2        | 0.1           |
| (1,808)  | 1:364:A:TRP:HZ2  | 1:353:A:SER:HB3  | 2        | 0.1           |
| (1,797)  | 1:364:A:TRP:HE3  | 1:385:A:TRP:HZ2  | 3        | 0.1           |
| (1,797)  | 1:364:A:TRP:HE3  | 1:385:A:TRP:HZ2  | 14       | 0.1           |
| (1,752)  | 1:361:A:LEU:HD11 | 1:353:A:SER:HA   | 11       | 0.1           |
| (1,752)  | 1:361:A:LEU:HD12 | 1:353:A:SER:HA   | 11       | 0.1           |
| (1,752)  | 1:361:A:LEU:HD13 | 1:353:A:SER:HA   | 11       | 0.1           |
| (1,752)  | 1:361:A:LEU:HD21 | 1:353:A:SER:HA   | 11       | 0.1           |
| (1,752)  | 1:361:A:LEU:HD22 | 1:353:A:SER:HA   | 11       | 0.1           |
| (1,752)  | 1:361:A:LEU:HD23 | 1:353:A:SER:HA   | 11       | 0.1           |
| (1,706)  | 1:358:A:TYR:HA   | 1:362:A:ASN:HB2  | 11       | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,706) | 1:358:A:TYR:HA  | 1:362:A:ASN:HB3 | 11       | 0.1           |
| (1,190) | 1:385:A:TRP:HH2 | 1:358:A:TYR:HA  | 22       | 0.1           |

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

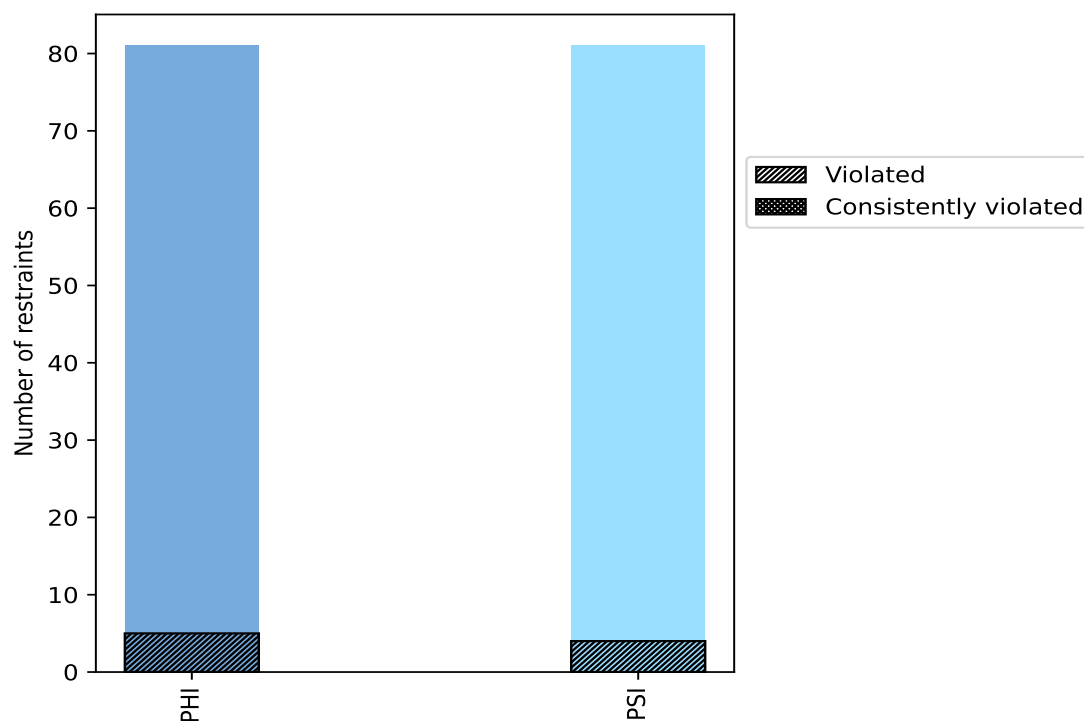
### 10.1 Summary of dihedral-angle violations [i](#)

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        | 81    | 50.0           | 5                     | 6.2            | 3.1            | 0                                  | 0.0            | 0.0            |
| PSI        | 81    | 50.0           | 4                     | 4.9            | 2.5            | 0                                  | 0.0            | 0.0            |
| Total      | 162   | 100.0          | 9                     | 5.6            | 5.6            | 0                                  | 0.0            | 0.0            |

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

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



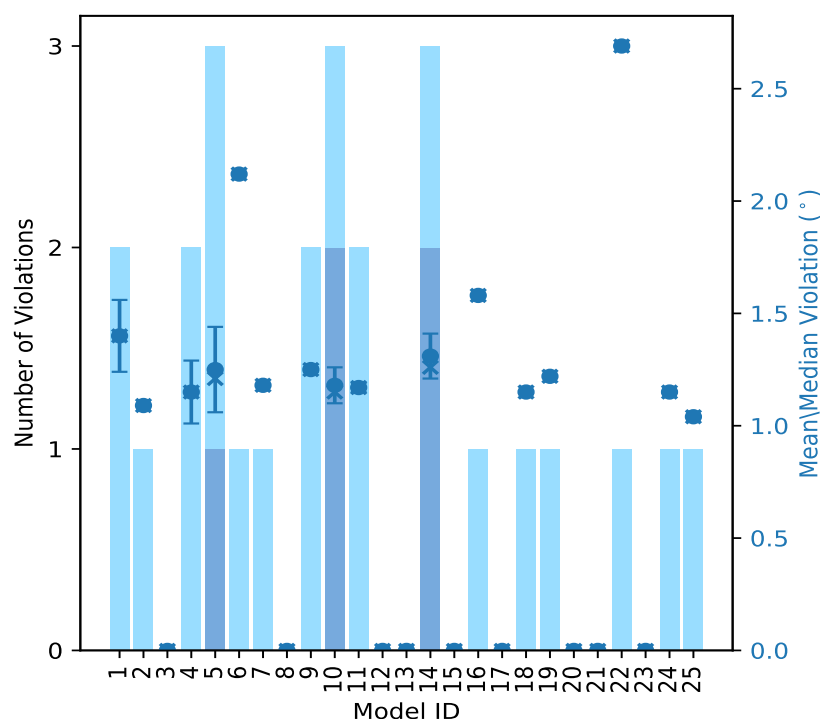
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 0                    | 2   | 2     | 1.4      | 1.55    | 0.16   | 1.4        |
| 2        | 0                    | 1   | 1     | 1.09     | 1.09    | 0.0    | 1.09       |
| 3        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 4        | 0                    | 2   | 2     | 1.15     | 1.29    | 0.14   | 1.15       |
| 5        | 1                    | 2   | 3     | 1.25     | 1.49    | 0.19   | 1.21       |
| 6        | 0                    | 1   | 1     | 2.12     | 2.12    | 0.0    | 2.12       |
| 7        | 0                    | 1   | 1     | 1.18     | 1.18    | 0.0    | 1.18       |
| 8        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 9        | 0                    | 2   | 2     | 1.25     | 1.26    | 0.01   | 1.25       |
| 10       | 2                    | 1   | 3     | 1.18     | 1.29    | 0.08   | 1.15       |
| 11       | 0                    | 2   | 2     | 1.17     | 1.19    | 0.02   | 1.17       |
| 12       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 13       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 14       | 2                    | 1   | 3     | 1.31     | 1.46    | 0.1    | 1.26       |
| 15       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 16       | 0                    | 1   | 1     | 1.58     | 1.58    | 0.0    | 1.58       |
| 17       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 18       | 0                    | 1   | 1     | 1.15     | 1.15    | 0.0    | 1.15       |
| 19       | 0                    | 1   | 1     | 1.22     | 1.22    | 0.0    | 1.22       |
| 20       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 21       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 22       | 0                    | 1   | 1     | 2.69     | 2.69    | 0.0    | 2.69       |
| 23       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 24       | 0                    | 1   | 1     | 1.15     | 1.15    | 0.0    | 1.15       |
| 25       | 0                    | 1   | 1     | 1.04     | 1.04    | 0.0    | 1.04       |

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



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

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

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

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %    |
| 5                             | 1   | 6     | 1                        | 4.0  |
| 0                             | 0   | 0     | 2                        | 8.0  |
| 0                             | 1   | 1     | 3                        | 12.0 |
| 0                             | 0   | 0     | 4                        | 16.0 |
| 0                             | 0   | 0     | 5                        | 20.0 |
| 0                             | 0   | 0     | 6                        | 24.0 |
| 0                             | 0   | 0     | 7                        | 28.0 |
| 0                             | 1   | 1     | 8                        | 32.0 |
| 0                             | 1   | 1     | 9                        | 36.0 |
| 0                             | 0   | 0     | 10                       | 40.0 |
| 0                             | 0   | 0     | 11                       | 44.0 |

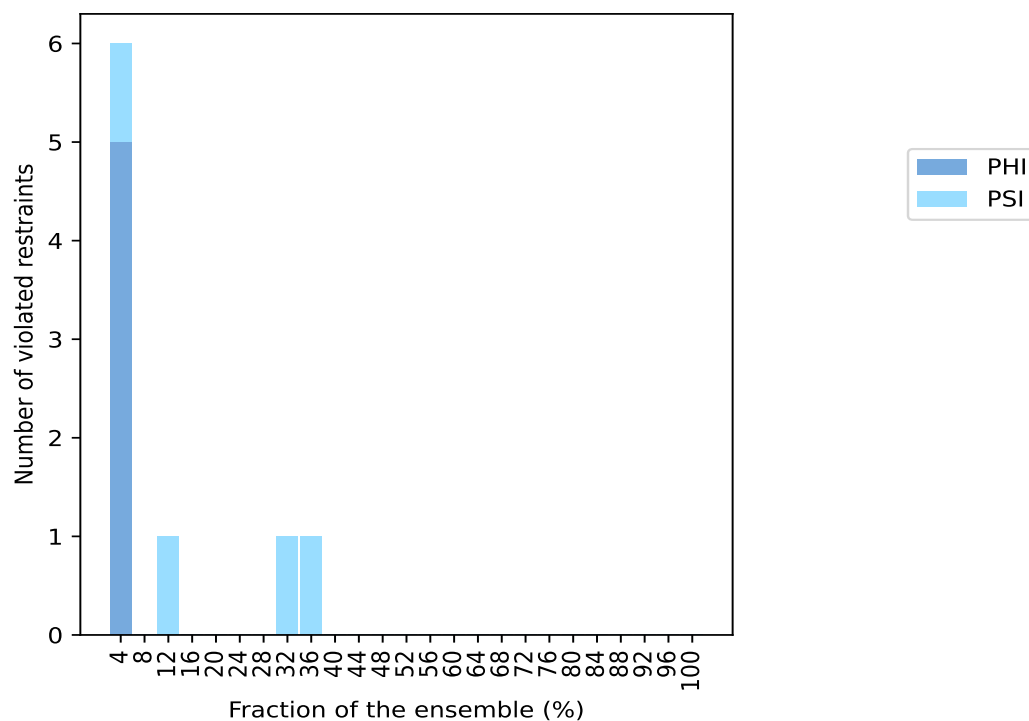
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0     | 12                       | 48.0  |
| 0                             | 0   | 0     | 13                       | 52.0  |
| 0                             | 0   | 0     | 14                       | 56.0  |
| 0                             | 0   | 0     | 15                       | 60.0  |
| 0                             | 0   | 0     | 16                       | 64.0  |
| 0                             | 0   | 0     | 17                       | 68.0  |
| 0                             | 0   | 0     | 18                       | 72.0  |
| 0                             | 0   | 0     | 19                       | 76.0  |
| 0                             | 0   | 0     | 20                       | 80.0  |
| 0                             | 0   | 0     | 21                       | 84.0  |
| 0                             | 0   | 0     | 22                       | 88.0  |
| 0                             | 0   | 0     | 23                       | 92.0  |
| 0                             | 0   | 0     | 24                       | 96.0  |
| 0                             | 0   | 0     | 25                       | 100.0 |

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

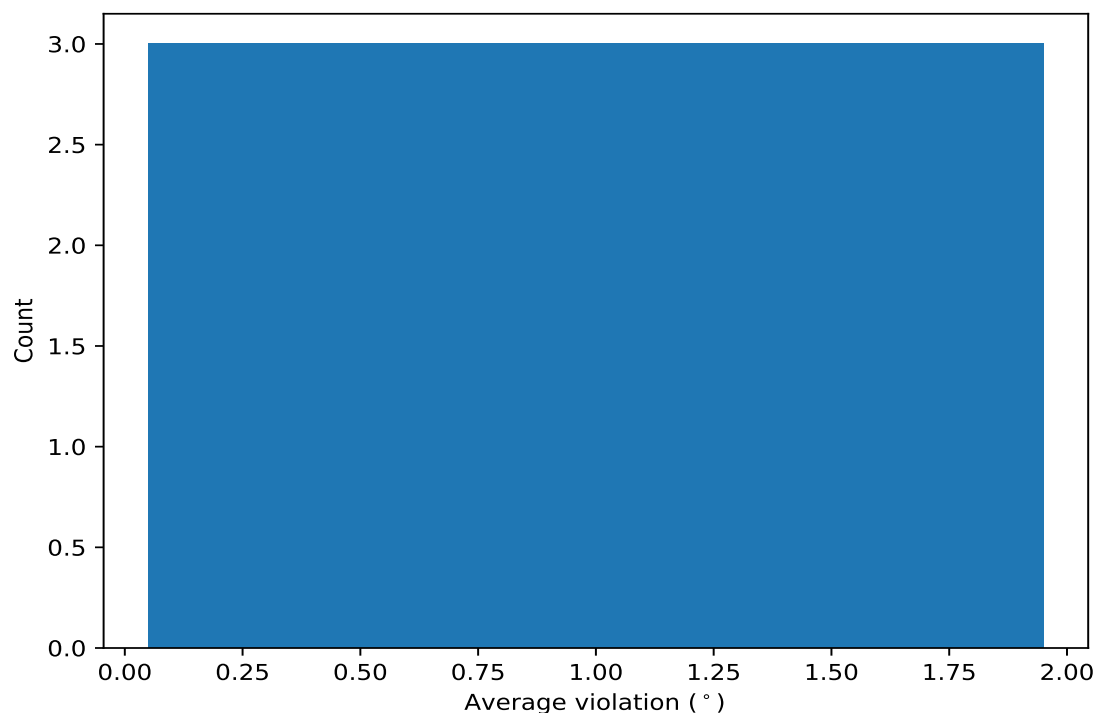
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

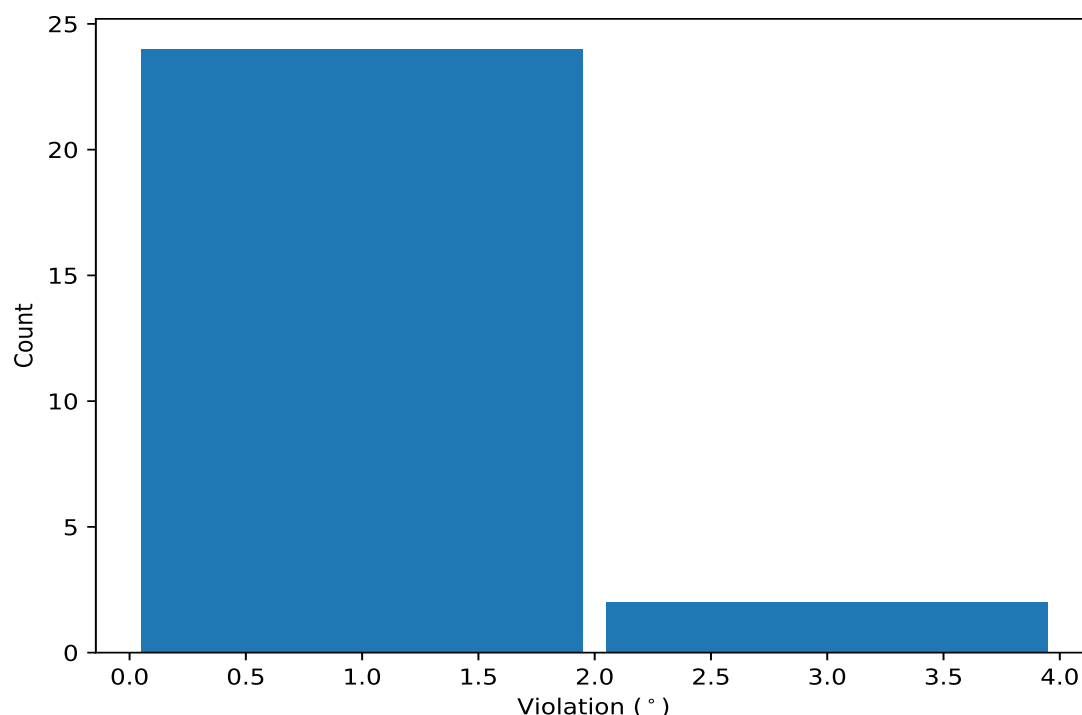
| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|---------------|---------------|---------------------|------|-----------------|--------|
| (1,70)  | 1:378:A:THR:N | 1:378:A:THR:CA | 1:378:A:THR:C | 1:379:A:THR:N | 9                   | 1.53 | 0.52            | 1.29   |
| (1,144) | 1:418:A:LYS:N | 1:418:A:LYS:CA | 1:418:A:LYS:C | 1:419:A:PRO:N | 8                   | 1.14 | 0.07            | 1.15   |
| (1,120) | 1:405:A:THR:N | 1:405:A:THR:CA | 1:405:A:THR:C | 1:406:A:LEU:N | 3                   | 1.22 | 0.0             | 1.22   |

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

## 10.5 All violated dihedral-angle restraints [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 (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,70)  | 1:378:A:THR:N | 1:378:A:THR:CA | 1:378:A:THR:C  | 1:379:A:THR:N | 22       | 2.69          |
| (1,70)  | 1:378:A:THR:N | 1:378:A:THR:CA | 1:378:A:THR:C  | 1:379:A:THR:N | 6        | 2.12          |
| (1,70)  | 1:378:A:THR:N | 1:378:A:THR:CA | 1:378:A:THR:C  | 1:379:A:THR:N | 16       | 1.58          |
| (1,70)  | 1:378:A:THR:N | 1:378:A:THR:CA | 1:378:A:THR:C  | 1:379:A:THR:N | 1        | 1.55          |
| (1,93)  | 1:391:A:GLY:C | 1:392:A:VAL:N  | 1:392:A:VAL:CA | 1:392:A:VAL:C | 5        | 1.49          |
| (1,23)  | 1:349:A:THR:C | 1:350:A:LEU:N  | 1:350:A:LEU:CA | 1:350:A:LEU:C | 14       | 1.46          |
| (1,70)  | 1:378:A:THR:N | 1:378:A:THR:CA | 1:378:A:THR:C  | 1:379:A:THR:N | 4        | 1.29          |
| (1,19)  | 1:347:A:HIS:C | 1:348:A:TYR:N  | 1:348:A:TYR:CA | 1:348:A:TYR:C | 10       | 1.29          |
| (1,144) | 1:418:A:LYS:N | 1:418:A:LYS:CA | 1:418:A:LYS:C  | 1:419:A:PRO:N | 9        | 1.26          |
| (1,85)  | 1:386:A:TYR:C | 1:387:A:VAL:N  | 1:387:A:VAL:CA | 1:387:A:VAL:C | 14       | 1.26          |
| (1,70)  | 1:378:A:THR:N | 1:378:A:THR:CA | 1:378:A:THR:C  | 1:379:A:THR:N | 9        | 1.25          |
| (1,138) | 1:415:A:PRO:N | 1:415:A:PRO:CA | 1:415:A:PRO:C  | 1:416:A:TRP:N | 1        | 1.24          |
| (1,120) | 1:405:A:THR:N | 1:405:A:THR:CA | 1:405:A:THR:C  | 1:406:A:LEU:N | 14       | 1.22          |
| (1,120) | 1:405:A:THR:N | 1:405:A:THR:CA | 1:405:A:THR:C  | 1:406:A:LEU:N | 19       | 1.22          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,120) | 1:405:A:THR:N | 1:405:A:THR:CA | 1:405:A:THR:C  | 1:406:A:LEU:N | 5        | 1.21          |
| (1,70)  | 1:378:A:THR:N | 1:378:A:THR:CA | 1:378:A:THR:C  | 1:379:A:THR:N | 11       | 1.19          |
| (1,144) | 1:418:A:LYS:N | 1:418:A:LYS:CA | 1:418:A:LYS:C  | 1:419:A:PRO:N | 7        | 1.18          |
| (1,144) | 1:418:A:LYS:N | 1:418:A:LYS:CA | 1:418:A:LYS:C  | 1:419:A:PRO:N | 11       | 1.16          |
| (1,144) | 1:418:A:LYS:N | 1:418:A:LYS:CA | 1:418:A:LYS:C  | 1:419:A:PRO:N | 10       | 1.15          |
| (1,144) | 1:418:A:LYS:N | 1:418:A:LYS:CA | 1:418:A:LYS:C  | 1:419:A:PRO:N | 18       | 1.15          |
| (1,144) | 1:418:A:LYS:N | 1:418:A:LYS:CA | 1:418:A:LYS:C  | 1:419:A:PRO:N | 24       | 1.15          |
| (1,73)  | 1:379:A:THR:C | 1:380:A:ARG:N  | 1:380:A:ARG:CA | 1:380:A:ARG:C | 10       | 1.1           |
| (1,144) | 1:418:A:LYS:N | 1:418:A:LYS:CA | 1:418:A:LYS:C  | 1:419:A:PRO:N | 2        | 1.09          |
| (1,70)  | 1:378:A:THR:N | 1:378:A:THR:CA | 1:378:A:THR:C  | 1:379:A:THR:N | 5        | 1.04          |
| (1,70)  | 1:378:A:THR:N | 1:378:A:THR:CA | 1:378:A:THR:C  | 1:379:A:THR:N | 25       | 1.04          |
| (1,144) | 1:418:A:LYS:N | 1:418:A:LYS:CA | 1:418:A:LYS:C  | 1:419:A:PRO:N | 4        | 1.01          |