



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 6YE5 / pdb\_00006ye5  
BMRB ID : 27532  
Title : Structure of ribosomal binding factor A RbfA of Staphylococcus aureus bacterium by NMR  
Authors : Blokhin, D.S.; Usachev, K.S.; Bikmullin, A.G.; Nurullina, L.; Garaeva, N.; Validov, S.; Klochkov, V.; Aganov, A.; Khusainov, I.; Yusupov, M.  
Deposited on : 2020-03-24

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

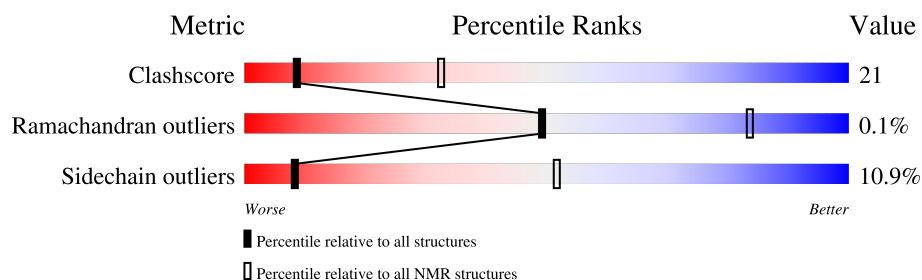
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 57%.

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     | 118    | <div> <div>42%</div> <div>25%</div> <div>.</div> <div>29%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                          |                   |              |
|--------------------------------------|--------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)    | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:4-A:78, A:88-A:96 (84) | 0.66              | 6            |

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 1 clusters. No single-model clusters were found.

| Cluster number | Models                        |
|----------------|-------------------------------|
| 1              | 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1939 atoms, of which 984 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribosome-binding factor A.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 118      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1939  | 597 | 984 | 167 | 184 | 7 |       |

There are 3 discrepancies between the modelled and reference sequences:

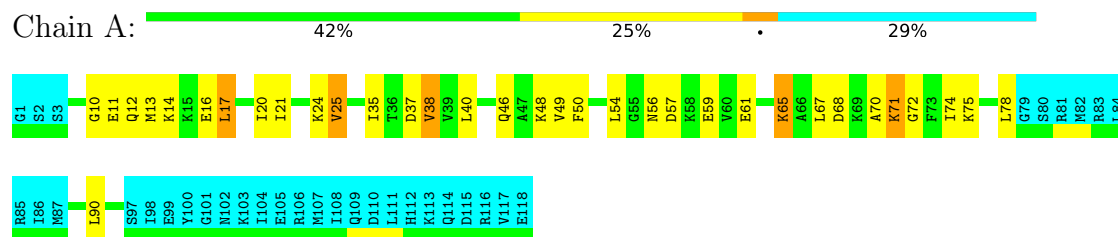
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | GLY      | -      | expression tag | UNP W8UYA0 |
| A     | 117     | VAL      | -      | expression tag | UNP W8UYA0 |
| A     | 118     | GLU      | -      | expression tag | UNP W8UYA0 |

## 4 Residue-property plots

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

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

- Molecule 1: Ribosome-binding factor A

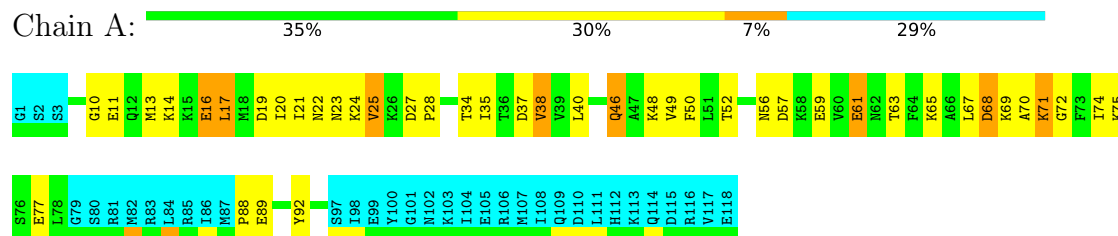


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

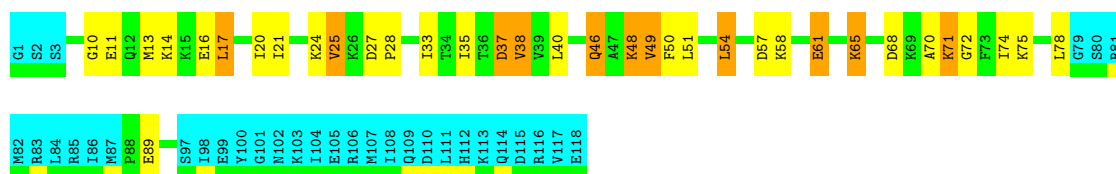
- Molecule 1: Ribosome-binding factor A



#### 4.2.2 Score per residue for model 2

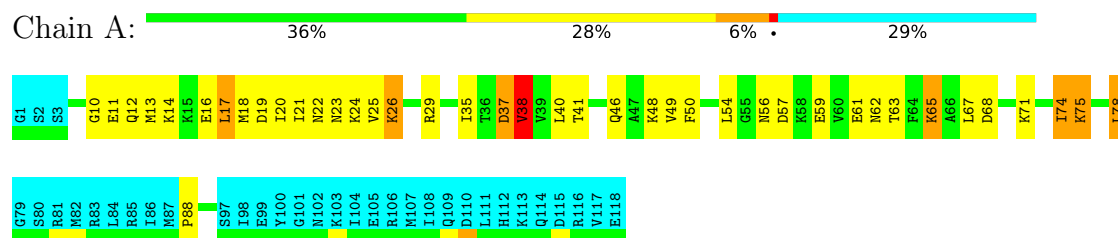
- Molecule 1: Ribosome-binding factor A





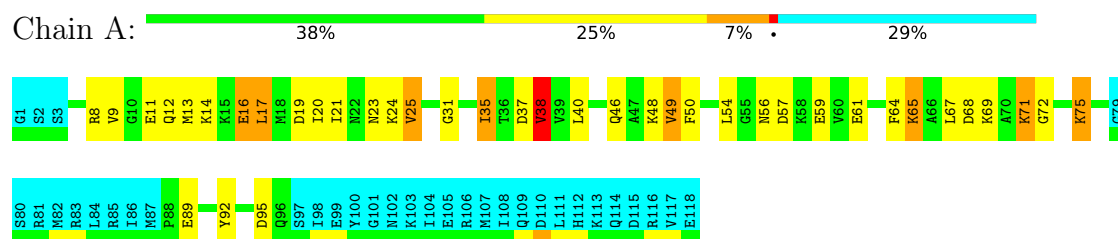
#### 4.2.3 Score per residue for model 3

- Molecule 1: Ribosome-binding factor A



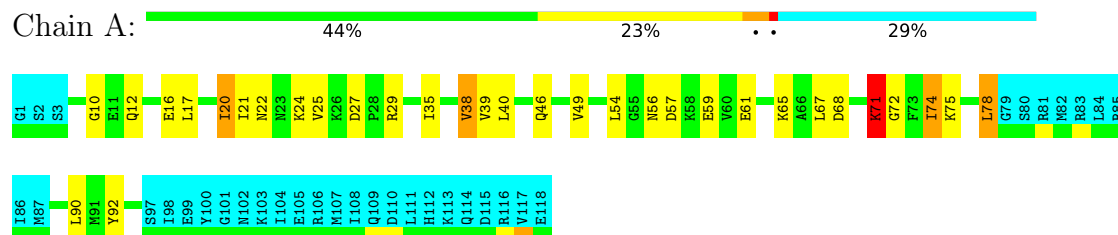
#### 4.2.4 Score per residue for model 4

- Molecule 1: Ribosome-binding factor A



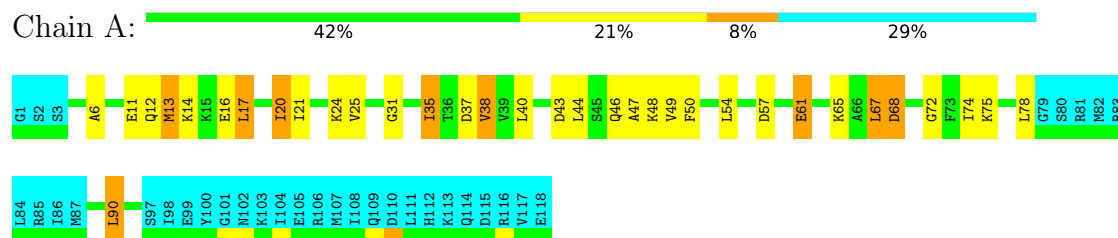
#### 4.2.5 Score per residue for model 5

- Molecule 1: Ribosome-binding factor A



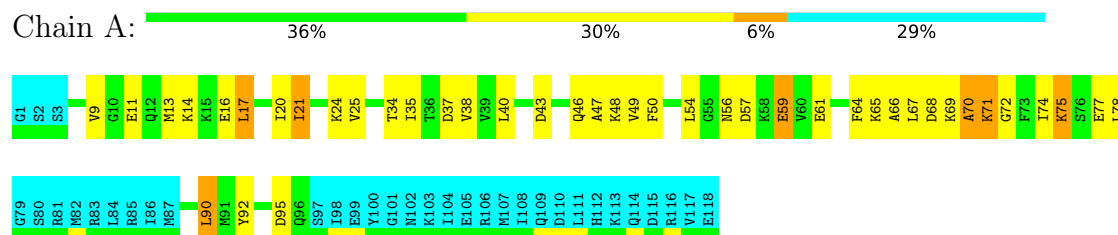
#### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Ribosome-binding factor A



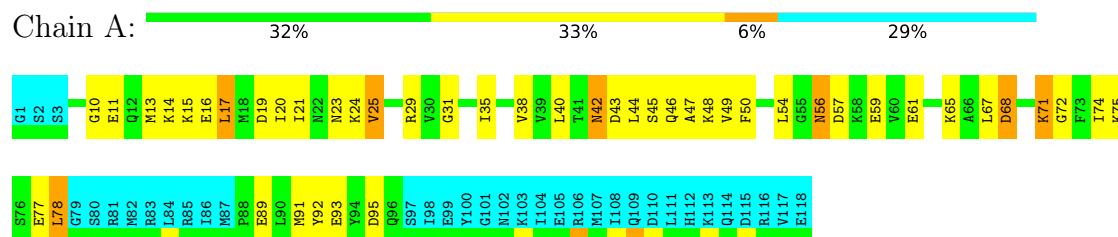
#### 4.2.7 Score per residue for model 7

- Molecule 1: Ribosome-binding factor A



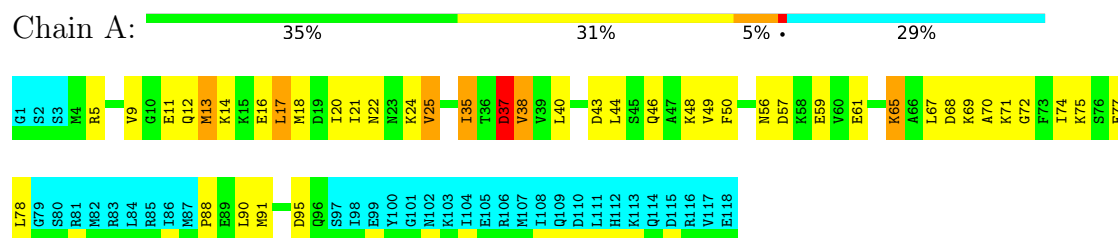
#### 4.2.8 Score per residue for model 8

- Molecule 1: Ribosome-binding factor A



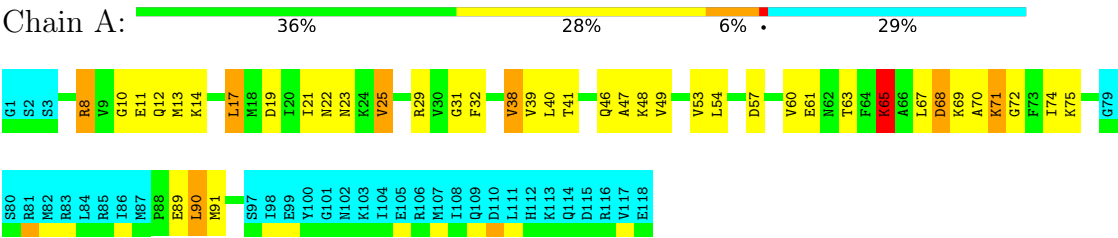
#### 4.2.9 Score per residue for model 9

- Molecule 1: Ribosome-binding factor A



4.2.10 Score per residue for model 10

● Molecule 1: Ribosome-binding factor A



## 5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| X-PLOR NIH    | structure calculation |         |

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                       | 831            |
| Number of shifts mapped to atoms             | 831            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 57%            |

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 1.10±0.03    | 3±1/683 ( 0.5± 0.2%) | 0.92±0.02   | 0±0/916 ( 0.0± 0.1%) |
| All | All   | 1.10         | 31/6830 ( 0.5%)      | 0.92        | 3/9160 ( 0.0%)       |

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

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 39  | VAL  | N-CA  | -7.59 | 1.36        | 1.46     | 5      | 2     |
| 1   | A     | 38  | VAL  | CA-C  | -7.43 | 1.43        | 1.52     | 5      | 3     |
| 1   | A     | 65  | LYS  | C-O   | -6.67 | 1.16        | 1.24     | 4      | 5     |
| 1   | A     | 71  | LYS  | C-O   | -6.43 | 1.16        | 1.24     | 7      | 2     |
| 1   | A     | 38  | VAL  | C-N   | -6.42 | 1.25        | 1.33     | 10     | 3     |
| 1   | A     | 61  | GLU  | C-O   | -6.17 | 1.16        | 1.24     | 1      | 3     |
| 1   | A     | 37  | ASP  | CA-C  | -5.93 | 1.47        | 1.53     | 2      | 2     |
| 1   | A     | 38  | VAL  | N-CA  | -5.87 | 1.38        | 1.46     | 2      | 6     |
| 1   | A     | 56  | ASN  | CA-C  | -5.70 | 1.45        | 1.53     | 8      | 1     |
| 1   | A     | 37  | ASP  | C-N   | -5.33 | 1.26        | 1.33     | 9      | 1     |
| 1   | A     | 48  | LYS  | CA-C  | -5.20 | 1.46        | 1.52     | 2      | 1     |
| 1   | A     | 49  | VAL  | N-CA  | -5.17 | 1.40        | 1.46     | 4      | 2     |

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

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
|     |       |     |      |        |       |             |          | Worst  | Total |
| 1   | A     | 42  | ASN  | N-CA-C | -6.18 | 103.25      | 111.96   | 8      | 1     |
| 1   | A     | 70  | ALA  | N-CA-C | -5.41 | 106.46      | 112.57   | 7      | 2     |

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     | 675   | 695      | 695      | 29±4    |
| All | All   | 6750  | 6950     | 6950     | 290     |

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 21.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:17:LEU:HG   | 1:A:49:VAL:HG21 | 0.83     | 1.51        | 9      | 7     |
| 1:A:38:VAL:HA   | 1:A:48:LYS:O    | 0.80     | 1.75        | 3      | 8     |
| 1:A:40:LEU:HA   | 1:A:46:GLN:O    | 0.76     | 1.80        | 7      | 10    |
| 1:A:14:LYS:HB2  | 1:A:38:VAL:HG22 | 0.70     | 1.62        | 9      | 5     |
| 1:A:71:LYS:O    | 1:A:75:LYS:HG3  | 0.70     | 1.86        | 5      | 1     |
| 1:A:16:GLU:O    | 1:A:20:ILE:HG13 | 0.69     | 1.88        | 7      | 3     |
| 1:A:68:ASP:O    | 1:A:71:LYS:HG3  | 0.68     | 1.87        | 5      | 3     |
| 1:A:65:LYS:HA   | 1:A:68:ASP:OD2  | 0.68     | 1.89        | 1      | 1     |
| 1:A:68:ASP:O    | 1:A:71:LYS:HB2  | 0.67     | 1.90        | 9      | 4     |
| 1:A:13:MET:O    | 1:A:17:LEU:HB2  | 0.66     | 1.89        | 3      | 9     |
| 1:A:71:LYS:O    | 1:A:74:ILE:HG22 | 0.66     | 1.90        | 5      | 1     |
| 1:A:16:GLU:O    | 1:A:20:ILE:HG12 | 0.65     | 1.92        | 9      | 4     |
| 1:A:57:ASP:O    | 1:A:61:GLU:HG2  | 0.65     | 1.91        | 8      | 4     |
| 1:A:11:GLU:O    | 1:A:14:LYS:HB3  | 0.64     | 1.92        | 7      | 6     |
| 1:A:42:ASN:HB3  | 1:A:46:GLN:NE2  | 0.64     | 2.07        | 8      | 1     |
| 1:A:21:ILE:HA   | 1:A:25:VAL:HG23 | 0.63     | 1.71        | 10     | 6     |
| 1:A:65:LYS:HA   | 1:A:68:ASP:OD1  | 0.63     | 1.93        | 10     | 3     |
| 1:A:20:ILE:HG21 | 1:A:78:LEU:HD21 | 0.61     | 1.71        | 6      | 1     |
| 1:A:8:ARG:O     | 1:A:12:GLN:HG3  | 0.61     | 1.95        | 4      | 2     |
| 1:A:14:LYS:HB2  | 1:A:38:VAL:CG2  | 0.60     | 2.26        | 9      | 5     |
| 1:A:35:ILE:H    | 1:A:35:ILE:HD13 | 0.60     | 1.55        | 9      | 3     |
| 1:A:61:GLU:O    | 1:A:65:LYS:HG3  | 0.60     | 1.96        | 1      | 7     |
| 1:A:10:GLY:O    | 1:A:38:VAL:HB   | 0.60     | 1.96        | 5      | 2     |
| 1:A:13:MET:HA   | 1:A:13:MET:HE2  | 0.60     | 1.73        | 3      | 1     |
| 1:A:71:LYS:HD2  | 1:A:72:GLY:N    | 0.60     | 2.11        | 2      | 2     |
| 1:A:74:ILE:O    | 1:A:78:LEU:HB2  | 0.60     | 1.96        | 5      | 3     |
| 1:A:20:ILE:O    | 1:A:24:LYS:HB2  | 0.59     | 1.96        | 3      | 9     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:66:ALA:O    | 1:A:70:ALA:HB3  | 0.59     | 1.96        | 7      | 1     |
| 1:A:71:LYS:O    | 1:A:75:LYS:HG2  | 0.59     | 1.98        | 8      | 4     |
| 1:A:13:MET:SD   | 1:A:78:LEU:HD11 | 0.59     | 2.37        | 2      | 1     |
| 1:A:10:GLY:O    | 1:A:14:LYS:HB2  | 0.58     | 1.99        | 8      | 1     |
| 1:A:67:LEU:HB3  | 1:A:92:TYR:CE1  | 0.58     | 2.34        | 7      | 2     |
| 1:A:40:LEU:HA   | 1:A:46:GLN:C    | 0.58     | 2.24        | 8      | 1     |
| 1:A:10:GLY:O    | 1:A:13:MET:HB2  | 0.57     | 1.99        | 3      | 3     |
| 1:A:9:VAL:HA    | 1:A:12:GLN:OE1  | 0.57     | 2.00        | 4      | 1     |
| 1:A:54:LEU:HD22 | 1:A:54:LEU:N    | 0.56     | 2.16        | 3      | 8     |
| 1:A:17:LEU:HA   | 1:A:20:ILE:HG22 | 0.56     | 1.78        | 6      | 1     |
| 1:A:56:ASN:N    | 1:A:59:GLU:HB2  | 0.56     | 2.16        | 3      | 7     |
| 1:A:61:GLU:O    | 1:A:65:LYS:HG2  | 0.56     | 2.00        | 7      | 3     |
| 1:A:25:VAL:HG21 | 1:A:74:ILE:HD11 | 0.56     | 1.78        | 9      | 2     |
| 1:A:14:LYS:HB3  | 1:A:38:VAL:HG22 | 0.55     | 1.77        | 3      | 2     |
| 1:A:72:GLY:HA2  | 1:A:75:LYS:CG   | 0.55     | 2.31        | 5      | 1     |
| 1:A:9:VAL:O     | 1:A:12:GLN:HG2  | 0.54     | 2.02        | 9      | 1     |
| 1:A:57:ASP:O    | 1:A:61:GLU:HG3  | 0.54     | 2.02        | 9      | 6     |
| 1:A:38:VAL:HG12 | 1:A:49:VAL:HA   | 0.54     | 1.79        | 7      | 7     |
| 1:A:11:GLU:O    | 1:A:14:LYS:HG2  | 0.54     | 2.03        | 4      | 2     |
| 1:A:37:ASP:O    | 1:A:50:PHE:HB2  | 0.53     | 2.03        | 2      | 7     |
| 1:A:14:LYS:HB3  | 1:A:38:VAL:CG2  | 0.53     | 2.34        | 4      | 2     |
| 1:A:43:ASP:HB2  | 1:A:46:GLN:OE1  | 0.53     | 2.03        | 9      | 1     |
| 1:A:43:ASP:HB3  | 1:A:46:GLN:OE1  | 0.52     | 2.04        | 7      | 1     |
| 1:A:27:ASP:N    | 1:A:28:PRO:HD3  | 0.51     | 2.21        | 2      | 2     |
| 1:A:19:ASP:O    | 1:A:23:ASN:HB2  | 0.51     | 2.06        | 10     | 5     |
| 1:A:70:ALA:O    | 1:A:74:ILE:HG12 | 0.51     | 2.06        | 2      | 3     |
| 1:A:29:ARG:NE   | 1:A:29:ARG:HA   | 0.51     | 2.21        | 10     | 2     |
| 1:A:71:LYS:CD   | 1:A:72:GLY:H    | 0.49     | 2.20        | 4      | 1     |
| 1:A:47:ALA:O    | 1:A:90:LEU:HA   | 0.49     | 2.07        | 10     | 3     |
| 1:A:69:LYS:C    | 1:A:71:LYS:H    | 0.49     | 2.15        | 9      | 1     |
| 1:A:72:GLY:HA2  | 1:A:75:LYS:HB2  | 0.49     | 1.84        | 10     | 6     |
| 1:A:41:THR:OG1  | 1:A:46:GLN:HB2  | 0.48     | 2.07        | 3      | 1     |
| 1:A:64:PHE:HA   | 1:A:67:LEU:CG   | 0.48     | 2.38        | 4      | 1     |
| 1:A:49:VAL:HB   | 1:A:91:MET:O    | 0.48     | 2.09        | 9      | 1     |
| 1:A:64:PHE:HA   | 1:A:67:LEU:HG   | 0.48     | 1.86        | 4      | 1     |
| 1:A:34:THR:HB   | 1:A:52:THR:CG2  | 0.48     | 2.38        | 1      | 1     |
| 1:A:12:GLN:O    | 1:A:16:GLU:HG2  | 0.48     | 2.07        | 6      | 2     |
| 1:A:5:ARG:NH1   | 1:A:44:LEU:HB2  | 0.48     | 2.24        | 9      | 1     |
| 1:A:63:THR:O    | 1:A:67:LEU:HG   | 0.47     | 2.09        | 10     | 1     |
| 1:A:43:ASP:O    | 1:A:44:LEU:HG   | 0.47     | 2.09        | 9      | 2     |
| 1:A:9:VAL:HB    | 1:A:40:LEU:HD11 | 0.47     | 1.86        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:43:ASP:OD2  | 1:A:45:SER:HB2  | 0.47     | 2.10        | 8      | 1     |
| 1:A:27:ASP:OD1  | 1:A:29:ARG:HG2  | 0.47     | 2.08        | 5      | 1     |
| 1:A:78:LEU:CD1  | 1:A:90:LEU:HG   | 0.47     | 2.39        | 7      | 1     |
| 1:A:38:VAL:CG1  | 1:A:49:VAL:HG22 | 0.47     | 2.39        | 9      | 1     |
| 1:A:21:ILE:HG13 | 1:A:22:ASN:N    | 0.47     | 2.25        | 5      | 2     |
| 1:A:90:LEU:H    | 1:A:90:LEU:HD13 | 0.47     | 1.69        | 10     | 2     |
| 1:A:11:GLU:O    | 1:A:15:LYS:HG2  | 0.47     | 2.10        | 8      | 1     |
| 1:A:71:LYS:O    | 1:A:75:LYS:N    | 0.47     | 2.44        | 7      | 2     |
| 1:A:17:LEU:HD13 | 1:A:49:VAL:CG2  | 0.47     | 2.40        | 5      | 1     |
| 1:A:67:LEU:HD13 | 1:A:92:TYR:CD1  | 0.46     | 2.45        | 4      | 1     |
| 1:A:20:ILE:HG12 | 1:A:77:GLU:CG   | 0.46     | 2.40        | 7      | 2     |
| 1:A:20:ILE:HG12 | 1:A:77:GLU:HG3  | 0.46     | 1.86        | 7      | 1     |
| 1:A:10:GLY:O    | 1:A:38:VAL:HG23 | 0.46     | 2.10        | 1      | 3     |
| 1:A:67:LEU:HD13 | 1:A:92:TYR:CG   | 0.46     | 2.45        | 4      | 1     |
| 1:A:67:LEU:HD22 | 1:A:92:TYR:CD2  | 0.45     | 2.46        | 4      | 1     |
| 1:A:75:LYS:N    | 1:A:75:LYS:HD3  | 0.45     | 2.26        | 4      | 1     |
| 1:A:67:LEU:HD13 | 1:A:92:TYR:CD2  | 0.45     | 2.47        | 8      | 2     |
| 1:A:20:ILE:CD1  | 1:A:77:GLU:HG3  | 0.45     | 2.41        | 9      | 1     |
| 1:A:72:GLY:HA2  | 1:A:75:LYS:HD3  | 0.45     | 1.89        | 5      | 1     |
| 1:A:17:LEU:O    | 1:A:21:ILE:HG22 | 0.45     | 2.12        | 1      | 2     |
| 1:A:67:LEU:O    | 1:A:71:LYS:HA   | 0.45     | 2.12        | 4      | 1     |
| 1:A:21:ILE:HD13 | 1:A:33:ILE:HG21 | 0.44     | 1.89        | 2      | 1     |
| 1:A:67:LEU:HD12 | 1:A:68:ASP:N    | 0.44     | 2.27        | 4      | 1     |
| 1:A:35:ILE:HD12 | 1:A:35:ILE:H    | 0.44     | 1.73        | 7      | 1     |
| 1:A:14:LYS:O    | 1:A:18:MET:HB2  | 0.44     | 2.12        | 3      | 1     |
| 1:A:67:LEU:O    | 1:A:74:ILE:HG13 | 0.44     | 2.12        | 6      | 2     |
| 1:A:17:LEU:O    | 1:A:20:ILE:HG22 | 0.44     | 2.13        | 5      | 1     |
| 1:A:35:ILE:HG23 | 1:A:49:VAL:HG13 | 0.44     | 1.88        | 8      | 1     |
| 1:A:65:LYS:O    | 1:A:69:LYS:N    | 0.44     | 2.48        | 9      | 3     |
| 1:A:31:GLY:HA3  | 1:A:54:LEU:HB2  | 0.43     | 1.89        | 10     | 4     |
| 1:A:35:ILE:HD12 | 1:A:35:ILE:N    | 0.43     | 2.29        | 7      | 1     |
| 1:A:21:ILE:C    | 1:A:21:ILE:HD13 | 0.43     | 2.38        | 7      | 1     |
| 1:A:11:GLU:CD   | 1:A:14:LYS:HD2  | 0.43     | 2.39        | 7      | 1     |
| 1:A:20:ILE:HD12 | 1:A:77:GLU:HG3  | 0.43     | 1.91        | 9      | 1     |
| 1:A:20:ILE:CD1  | 1:A:78:LEU:HG   | 0.43     | 2.44        | 7      | 1     |
| 1:A:58:LYS:O    | 1:A:61:GLU:HB2  | 0.43     | 2.14        | 2      | 1     |
| 1:A:61:GLU:O    | 1:A:65:LYS:N    | 0.43     | 2.51        | 7      | 1     |
| 1:A:41:THR:CG2  | 1:A:46:GLN:HB2  | 0.43     | 2.44        | 10     | 1     |
| 1:A:48:LYS:HE3  | 1:A:50:PHE:CE1  | 0.42     | 2.49        | 8      | 1     |
| 1:A:32:PHE:O    | 1:A:53:VAL:HA   | 0.42     | 2.14        | 10     | 1     |
| 1:A:13:MET:HE3  | 1:A:78:LEU:HD12 | 0.42     | 1.92        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:71:LYS:HD2  | 1:A:72:GLY:H    | 0.42     | 1.74        | 1      | 1     |
| 1:A:59:GLU:O    | 1:A:62:ASN:HB3  | 0.42     | 2.15        | 3      | 1     |
| 1:A:17:LEU:O    | 1:A:21:ILE:HG12 | 0.42     | 2.14        | 10     | 2     |
| 1:A:10:GLY:CA   | 1:A:40:LEU:HD23 | 0.42     | 2.45        | 3      | 1     |
| 1:A:48:LYS:HB2  | 1:A:91:MET:HE3  | 0.42     | 1.90        | 8      | 1     |
| 1:A:38:VAL:HG23 | 1:A:38:VAL:O    | 0.42     | 2.15        | 1      | 1     |
| 1:A:67:LEU:HD23 | 1:A:92:TYR:CD2  | 0.42     | 2.50        | 5      | 1     |
| 1:A:26:LYS:O    | 1:A:26:LYS:HD2  | 0.41     | 2.15        | 3      | 1     |
| 1:A:17:LEU:HG   | 1:A:49:VAL:CG2  | 0.41     | 2.44        | 4      | 1     |
| 1:A:38:VAL:O    | 1:A:38:VAL:HG23 | 0.41     | 2.15        | 9      | 2     |
| 1:A:90:LEU:C    | 1:A:90:LEU:HD22 | 0.41     | 2.40        | 7      | 1     |
| 1:A:71:LYS:C    | 1:A:75:LYS:HG3  | 0.41     | 2.41        | 5      | 1     |
| 1:A:72:GLY:HA2  | 1:A:75:LYS:CD   | 0.41     | 2.46        | 5      | 1     |
| 1:A:20:ILE:HD12 | 1:A:77:GLU:CG   | 0.41     | 2.45        | 8      | 1     |
| 1:A:40:LEU:HG   | 1:A:47:ALA:HB2  | 0.41     | 1.93        | 8      | 1     |
| 1:A:48:LYS:HA   | 1:A:91:MET:HB3  | 0.41     | 1.91        | 9      | 1     |
| 1:A:35:ILE:H    | 1:A:35:ILE:CD1  | 0.41     | 2.26        | 9      | 1     |
| 1:A:6:ALA:HA    | 1:A:40:LEU:HB3  | 0.41     | 1.92        | 6      | 1     |
| 1:A:57:ASP:O    | 1:A:60:VAL:HB   | 0.40     | 2.17        | 10     | 1     |
| 1:A:69:LYS:C    | 1:A:69:LYS:HD2  | 0.40     | 2.41        | 1      | 1     |
| 1:A:69:LYS:HD3  | 1:A:69:LYS:C    | 0.40     | 2.40        | 4      | 1     |
| 1:A:18:MET:O    | 1:A:22:ASN:HB2  | 0.40     | 2.15        | 9      | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed       | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|----------------|--------------|------------|------------|-------------|----|
| 1   | A     | 84/118 (71%)   | 81±2 (96±2%) | 3±2 (4±2%) | 0±0 (0±0%) | 49          | 83 |
| All | All   | 840/1180 (71%) | 806 (96%)    | 33 (4%)    | 1 (0%)     | 49          | 83 |

All 1 unique Ramachandran outliers are listed below.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 71  | LYS  | 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     | 76/107 (71%)   | 68±2 (89±3%) | 8±2 (11±3%) | <b>8</b> 52 |
| All | All   | 760/1070 (71%) | 677 (89%)    | 83 (11%)    | <b>8</b> 52 |

All 32 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     | 25  | VAL  | 10             |
| 1   | A     | 17  | LEU  | 9              |
| 1   | A     | 35  | ILE  | 7              |
| 1   | A     | 68  | ASP  | 5              |
| 1   | A     | 71  | LYS  | 5              |
| 1   | A     | 78  | LEU  | 4              |
| 1   | A     | 90  | LEU  | 4              |
| 1   | A     | 16  | GLU  | 3              |
| 1   | A     | 75  | LYS  | 3              |
| 1   | A     | 22  | ASN  | 2              |
| 1   | A     | 46  | GLN  | 2              |
| 1   | A     | 63  | THR  | 2              |
| 1   | A     | 12  | GLN  | 2              |
| 1   | A     | 21  | ILE  | 2              |
| 1   | A     | 38  | VAL  | 2              |
| 1   | A     | 67  | LEU  | 2              |
| 1   | A     | 74  | ILE  | 2              |
| 1   | A     | 20  | ILE  | 2              |
| 1   | A     | 13  | MET  | 2              |
| 1   | A     | 51  | LEU  | 1              |
| 1   | A     | 54  | LEU  | 1              |
| 1   | A     | 26  | LYS  | 1              |
| 1   | A     | 29  | ARG  | 1              |
| 1   | A     | 34  | THR  | 1              |
| 1   | A     | 59  | GLU  | 1              |
| 1   | A     | 64  | PHE  | 1              |
| 1   | A     | 69  | LYS  | 1              |
| 1   | A     | 44  | LEU  | 1              |
| 1   | A     | 95  | ASP  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 37  | ASP  | 1              |
| 1   | A     | 8   | ARG  | 1              |
| 1   | A     | 65  | LYS  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 57% for the well-defined parts and 49% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 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                  | 831 |
| Number of shifts mapped to atoms        | 831 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 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      | $-0.47 \pm 0.17$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 90       | $0.15 \pm 0.11$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 99       | $-0.12 \pm 0.12$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 94       | $-0.16 \pm 0.29$                | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 57%, i.e. 679 atoms were assigned a chemical shift out of a possible 1188. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 389/420 (93%) | 154/170 (91%) | 160/168 (95%)   | 75/82 (91%)     |
| Sidechain | 278/710 (39%) | 157/458 (34%) | 114/225 (51%)   | 7/27 (26%)      |

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|          | <b>Total</b>   | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 12/58 (21%)    | 12/28 (43%)          | 0/30 (0%)             | 0/0 (—%)              |
| Overall  | 679/1188 (57%) | 323/656 (49%)        | 274/423 (65%)         | 82/109 (75%)          |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 49%, i.e. 831 atoms were assigned a chemical shift out of a possible 1686. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>   | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 488/593 (82%)  | 194/241 (80%)        | 200/236 (85%)         | 94/116 (81%)          |
| Sidechain | 329/1018 (32%) | 182/655 (28%)        | 139/316 (44%)         | 8/47 (17%)            |
| Aromatic  | 14/75 (19%)    | 14/36 (39%)          | 0/37 (0%)             | 0/2 (0%)              |
| Overall   | 831/1686 (49%) | 390/932 (42%)        | 339/589 (58%)         | 102/165 (62%)         |

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

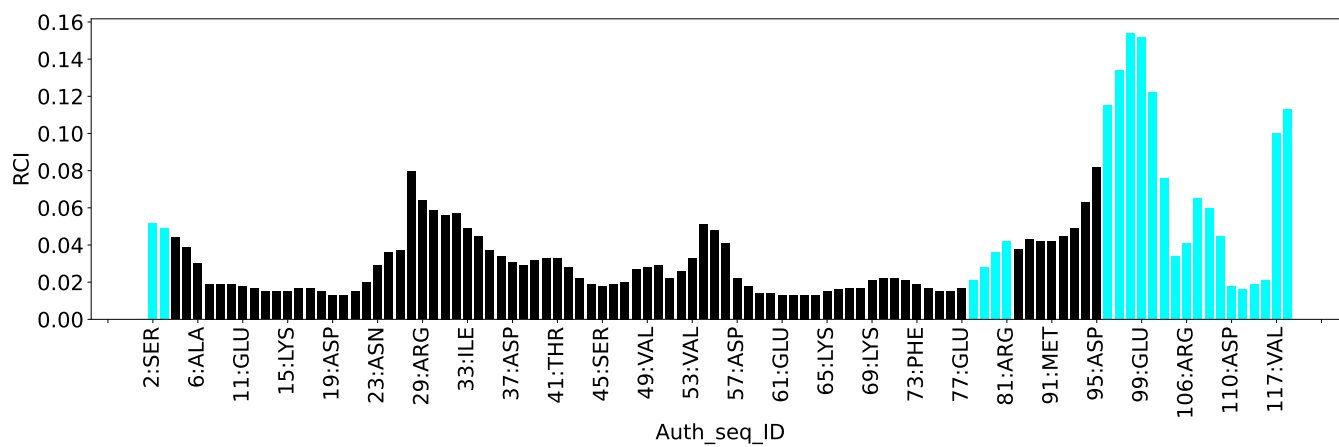
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 29  | ARG  | NE   | 111.60     | 76.53 – 92.65       | 16.8    |

#### 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                                | 3196  |
| Intra-residue ( $ i-j =0$ )                              | 928   |
| Sequential ( $ i-j =1$ )                                 | 874   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 697   |
| Long range ( $ i-j \geq 5$ )                             | 530   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 167   |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 220   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 28.9  |
| Number of long range restraints per residue <sup>1</sup> | 5.0   |

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

#### 8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 65.7                                   | 0.2     |
| 0.2-0.5 (Medium) | 54.7                                   | 0.5     |
| >0.5 (Large)     | 12.2                                   | 1.12    |

### 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)   | 17.6                                   | 8.97    |
| 10.0-20.0 (Medium) | 0.3                                    | 18.46   |
| >20.0 (Large)      | 1.2                                    | 122.43  |

## 9 Distance violation analysis ⓘ

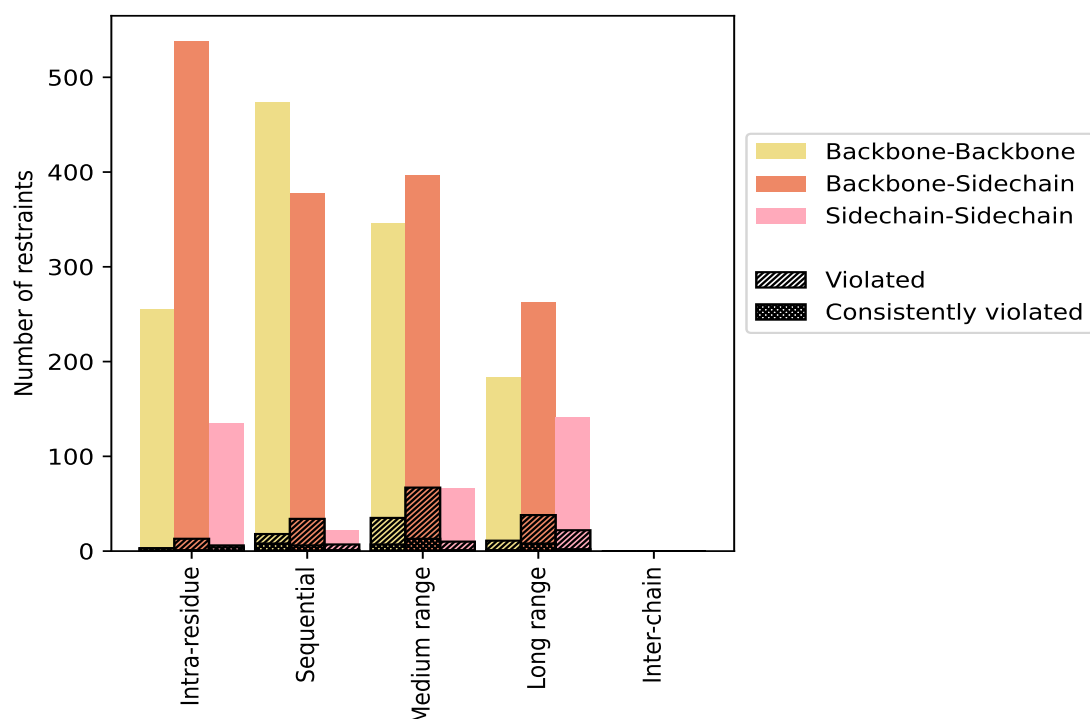
### 9.1 Summary of distance violations ⓘ

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>928</b>  | <b>29.0</b>    | <b>22</b>             | <b>2.4</b>     | <b>0.7</b>     | <b>8</b>                           | <b>0.9</b>     | <b>0.3</b>     |
| Backbone-Backbone                                                           | 255         | 8.0            | 3                     | 1.2            | 0.1            | 3                                  | 1.2            | 0.1            |
| Backbone-Sidechain                                                          | 538         | 16.8           | 13                    | 2.4            | 0.4            | 1                                  | 0.2            | 0.0            |
| Sidechain-Sidechain                                                         | 135         | 4.2            | 6                     | 4.4            | 0.2            | 4                                  | 3.0            | 0.1            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>874</b>  | <b>27.3</b>    | <b>59</b>             | <b>6.8</b>     | <b>1.8</b>     | <b>15</b>                          | <b>1.7</b>     | <b>0.5</b>     |
| Backbone-Backbone                                                           | 474         | 14.8           | 18                    | 3.8            | 0.6            | 8                                  | 1.7            | 0.3            |
| Backbone-Sidechain                                                          | 378         | 11.8           | 34                    | 9.0            | 1.1            | 6                                  | 1.6            | 0.2            |
| Sidechain-Sidechain                                                         | 22          | 0.7            | 7                     | 31.8           | 0.2            | 1                                  | 4.5            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>697</b>  | <b>21.8</b>    | <b>92</b>             | <b>13.2</b>    | <b>2.9</b>     | <b>19</b>                          | <b>2.7</b>     | <b>0.6</b>     |
| Backbone-Backbone                                                           | 346         | 10.8           | 35                    | 10.1           | 1.1            | 7                                  | 2.0            | 0.2            |
| Backbone-Sidechain                                                          | 285         | 8.9            | 47                    | 16.5           | 1.5            | 11                                 | 3.9            | 0.3            |
| Sidechain-Sidechain                                                         | 66          | 2.1            | 10                    | 15.2           | 0.3            | 1                                  | 1.5            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>530</b>  | <b>16.6</b>    | <b>69</b>             | <b>13.0</b>    | <b>2.2</b>     | <b>11</b>                          | <b>2.1</b>     | <b>0.3</b>     |
| Backbone-Backbone                                                           | 183         | 5.7            | 11                    | 6.0            | 0.3            | 1                                  | 0.5            | 0.0            |
| Backbone-Sidechain                                                          | 206         | 6.4            | 36                    | 17.5           | 1.1            | 8                                  | 3.9            | 0.3            |
| Sidechain-Sidechain                                                         | 141         | 4.4            | 22                    | 15.6           | 0.7            | 2                                  | 1.4            | 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>167</b>  | <b>5.2</b>     | <b>22</b>             | <b>13.2</b>    | <b>0.7</b>     | <b>2</b>                           | <b>1.2</b>     | <b>0.1</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>3196</b> | <b>100.0</b>   | <b>264</b>            | <b>8.3</b>     | <b>8.3</b>     | <b>55</b>                          | <b>1.7</b>     | <b>1.7</b>     |
| Backbone-Backbone                                                           | 1258        | 39.4           | 67                    | 5.3            | 2.1            | 19                                 | 1.5            | 0.6            |
| Backbone-Sidechain                                                          | 1574        | 49.2           | 152                   | 9.7            | 4.8            | 28                                 | 1.8            | 0.9            |
| Sidechain-Sidechain                                                         | 364         | 11.4           | 45                    | 12.4           | 1.4            | 8                                  | 2.2            | 0.3            |

<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

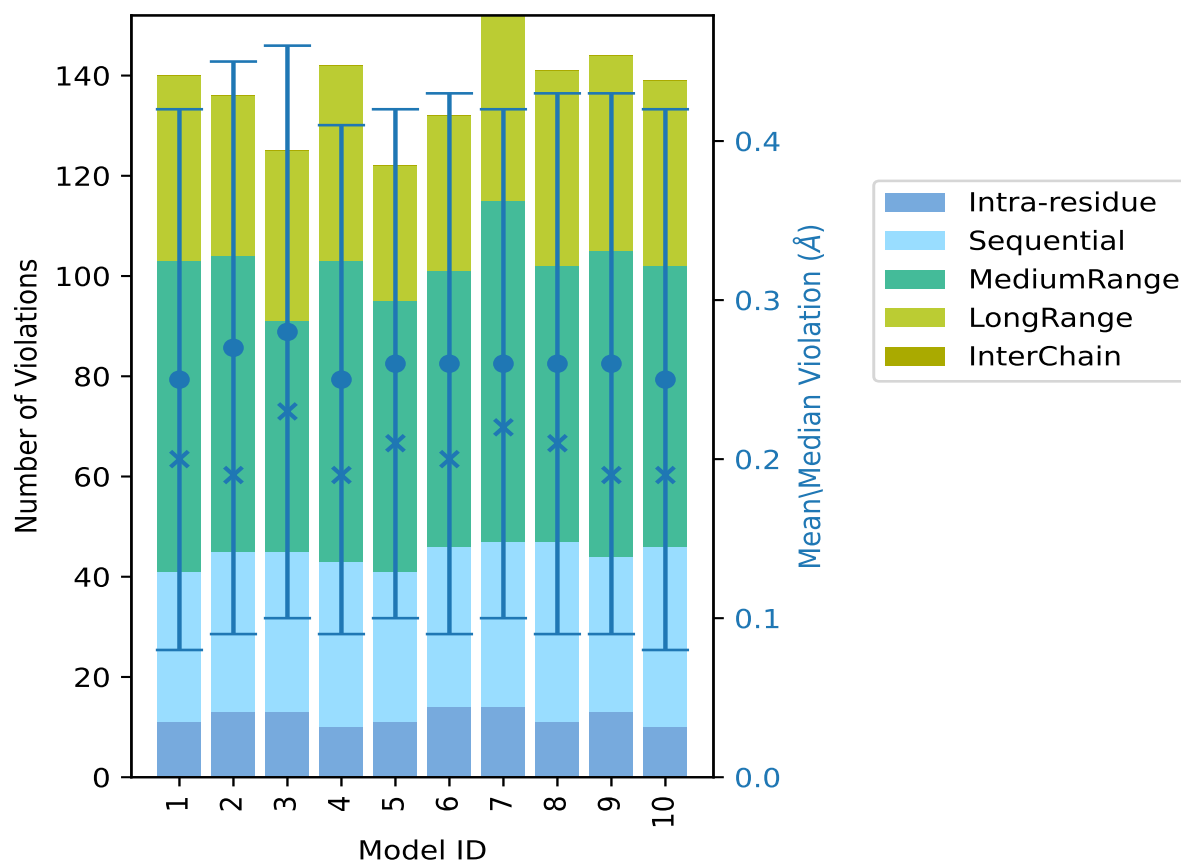
## 9.2 Distance violation statistics for each model [i](#)

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        | 11                   | 30              | 62              | 37              | 0               | 140   | 0.25     | 0.98    | 0.17                | 0.2        |
| 2        | 13                   | 32              | 59              | 32              | 0               | 136   | 0.27     | 0.99    | 0.18                | 0.19       |
| 3        | 13                   | 32              | 46              | 34              | 0               | 125   | 0.28     | 1.12    | 0.18                | 0.23       |
| 4        | 10                   | 33              | 60              | 39              | 0               | 142   | 0.25     | 0.99    | 0.16                | 0.19       |
| 5        | 11                   | 30              | 54              | 27              | 0               | 122   | 0.26     | 1.02    | 0.16                | 0.21       |
| 6        | 14                   | 32              | 55              | 31              | 0               | 132   | 0.26     | 0.98    | 0.17                | 0.2        |
| 7        | 14                   | 33              | 68              | 37              | 0               | 152   | 0.26     | 0.97    | 0.16                | 0.22       |
| 8        | 11                   | 36              | 55              | 39              | 0               | 141   | 0.26     | 1.0     | 0.17                | 0.21       |
| 9        | 13                   | 31              | 61              | 39              | 0               | 144   | 0.26     | 0.97    | 0.17                | 0.19       |
| 10       | 10                   | 36              | 56              | 37              | 0               | 139   | 0.25     | 1.01    | 0.17                | 0.19       |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model [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, 2787(IR:906, SQ:815, MR:605, LR:461, 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>       | %    |
| 4                             | 14              | 15              | 16              | 0               | 49    | 1                        | 10.0 |
| 4                             | 8               | 12              | 7               | 0               | 31    | 2                        | 20.0 |
| 3                             | 2               | 14              | 7               | 0               | 26    | 3                        | 30.0 |

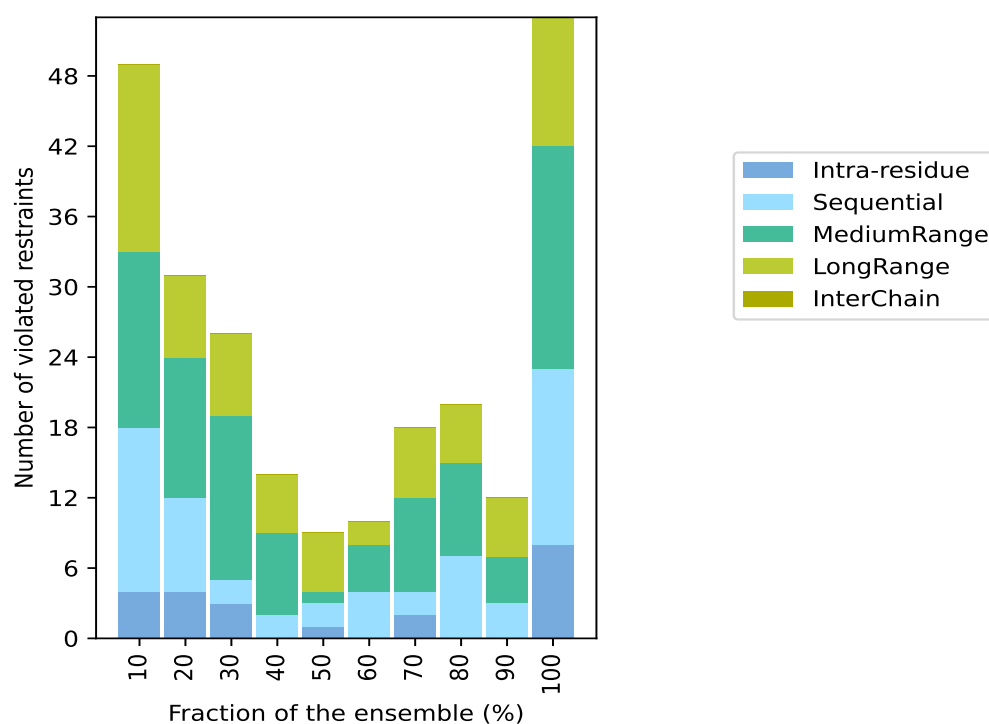
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| 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                             | 2               | 7               | 5               | 0               | 14    | 4                        | 40.0  |
| 1                             | 2               | 1               | 5               | 0               | 9     | 5                        | 50.0  |
| 0                             | 4               | 4               | 2               | 0               | 10    | 6                        | 60.0  |
| 2                             | 2               | 8               | 6               | 0               | 18    | 7                        | 70.0  |
| 0                             | 7               | 8               | 5               | 0               | 20    | 8                        | 80.0  |
| 0                             | 3               | 4               | 5               | 0               | 12    | 9                        | 90.0  |
| 8                             | 15              | 19              | 11              | 0               | 53    | 10                       | 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](#)

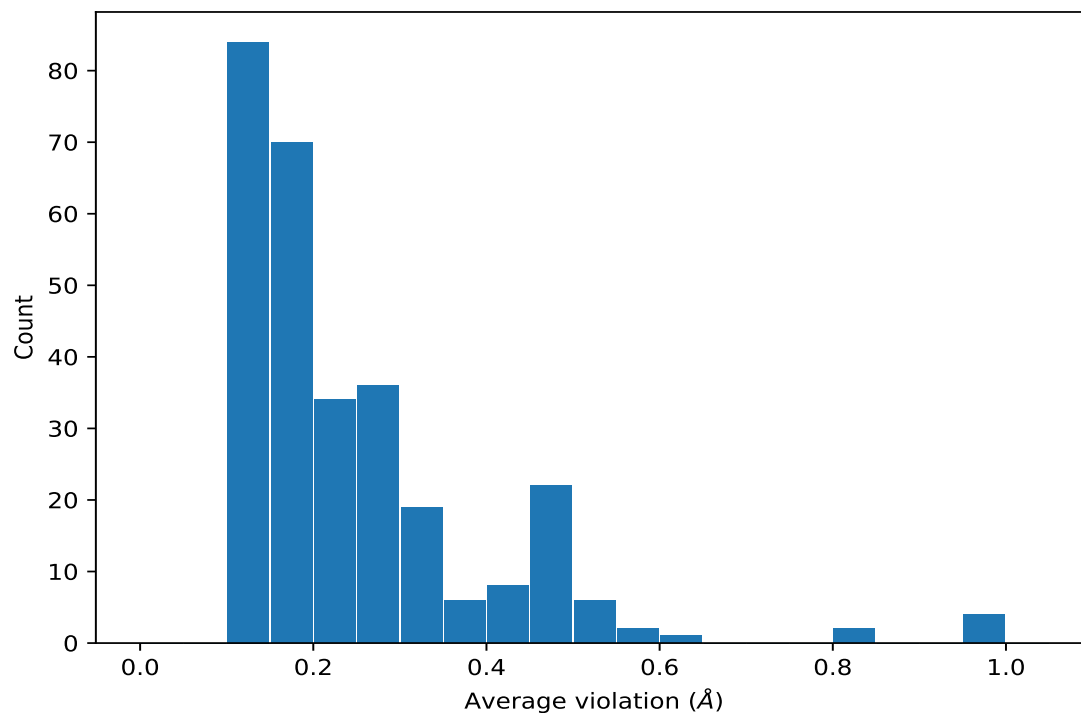


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,3028) | 1:113:A:LYS:H   | 1:113:A:LYS:HA  | 10                  | 0.98     | 0.01                | 0.98       |
| (2,1984) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 10                  | 0.81     | 0.03                | 0.8        |
| (2,1792) | 1:3:A:SER:H     | 1:3:A:SER:HA    | 10                  | 0.63     | 0.03                | 0.64       |
| (2,2247) | 1:11:A:GLU:H    | 1:12:A:GLN:HA   | 10                  | 0.58     | 0.03                | 0.58       |
| (2,950)  | 1:111:A:LEU:HB2 | 1:110:A:ASP:HB2 | 10                  | 0.55     | 0.2                 | 0.46       |
| (2,2859) | 1:65:A:LYS:H    | 1:61:A:GLU:HB2  | 10                  | 0.54     | 0.03                | 0.55       |
| (2,2869) | 1:68:A:ASP:H    | 1:92:A:TYR:HB3  | 10                  | 0.53     | 0.11                | 0.56       |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD21 | 10                  | 0.49     | 0.06                | 0.52       |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD22 | 10                  | 0.49     | 0.06                | 0.52       |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD23 | 10                  | 0.49     | 0.06                | 0.52       |
| (2,1797) | 1:9:A:VAL:H     | 1:9:A:VAL:HA    | 10                  | 0.49     | 0.02                | 0.49       |
| (2,1098) | 1:38:A:VAL:HG21 | 1:17:A:LEU:H    | 10                  | 0.48     | 0.08                | 0.48       |
| (2,1098) | 1:38:A:VAL:HG22 | 1:17:A:LEU:H    | 10                  | 0.48     | 0.08                | 0.48       |
| (2,1098) | 1:38:A:VAL:HG23 | 1:17:A:LEU:H    | 10                  | 0.48     | 0.08                | 0.48       |
| (2,1105) | 1:39:A:VAL:HG21 | 1:37:A:ASP:HB2  | 10                  | 0.47     | 0.09                | 0.44       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,1105) | 1:39:A:VAL:HG22 | 1:37:A:ASP:HB2  | 10                  | 0.47     | 0.09                | 0.44       |
| (2,1105) | 1:39:A:VAL:HG23 | 1:37:A:ASP:HB2  | 10                  | 0.47     | 0.09                | 0.44       |
| (2,2877) | 1:69:A:LYS:H    | 1:65:A:LYS:HB2  | 10                  | 0.47     | 0.07                | 0.48       |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB1  | 10                  | 0.47     | 0.03                | 0.46       |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB2  | 10                  | 0.47     | 0.03                | 0.46       |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB3  | 10                  | 0.47     | 0.03                | 0.46       |
| (2,2842) | 1:61:A:GLU:H    | 1:59:A:GLU:HB2  | 10                  | 0.46     | 0.03                | 0.46       |
| (2,1096) | 1:38:A:VAL:HG21 | 1:37:A:ASP:HA   | 10                  | 0.45     | 0.09                | 0.46       |
| (2,1096) | 1:38:A:VAL:HG22 | 1:37:A:ASP:HA   | 10                  | 0.45     | 0.09                | 0.46       |
| (2,1096) | 1:38:A:VAL:HG23 | 1:37:A:ASP:HA   | 10                  | 0.45     | 0.09                | 0.46       |
| (2,1102) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HA   | 10                  | 0.45     | 0.06                | 0.42       |
| (2,1102) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HA   | 10                  | 0.45     | 0.06                | 0.42       |
| (2,1102) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HA   | 10                  | 0.45     | 0.06                | 0.42       |
| (2,601)  | 1:38:A:VAL:HG21 | 1:48:A:LYS:H    | 10                  | 0.42     | 0.12                | 0.46       |
| (2,601)  | 1:38:A:VAL:HG22 | 1:48:A:LYS:H    | 10                  | 0.42     | 0.12                | 0.46       |
| (2,601)  | 1:38:A:VAL:HG23 | 1:48:A:LYS:H    | 10                  | 0.42     | 0.12                | 0.46       |
| (2,2831) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 10                  | 0.41     | 0.03                | 0.4        |
| (2,1765) | 1:109:A:GLN:H   | 1:110:A:ASP:HB3 | 10                  | 0.4      | 0.08                | 0.4        |
| (2,2928) | 1:79:A:GLY:H    | 1:75:A:LYS:HB2  | 10                  | 0.38     | 0.04                | 0.38       |
| (2,604)  | 1:38:A:VAL:HG21 | 1:47:A:ALA:HA   | 10                  | 0.38     | 0.12                | 0.38       |
| (2,604)  | 1:38:A:VAL:HG22 | 1:47:A:ALA:HA   | 10                  | 0.38     | 0.12                | 0.38       |
| (2,604)  | 1:38:A:VAL:HG23 | 1:47:A:ALA:HA   | 10                  | 0.38     | 0.12                | 0.38       |
| (2,1143) | 1:50:A:PHE:HB3  | 1:37:A:ASP:HB3  | 10                  | 0.36     | 0.06                | 0.37       |
| (2,1576) | 1:58:A:LYS:H    | 1:61:A:GLU:HB2  | 10                  | 0.35     | 0.05                | 0.35       |
| (2,932)  | 1:109:A:GLN:HB2 | 1:107:A:MET:HA  | 10                  | 0.34     | 0.13                | 0.33       |
| (2,2358) | 1:41:A:THR:H    | 1:46:A:GLN:HA   | 10                  | 0.34     | 0.04                | 0.34       |
| (2,2881) | 1:70:A:ALA:H    | 1:71:A:LYS:HB3  | 10                  | 0.33     | 0.1                 | 0.32       |
| (2,1291) | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 10                  | 0.31     | 0.03                | 0.32       |
| (2,1924) | 1:45:A:SER:H    | 1:46:A:GLN:HA   | 10                  | 0.31     | 0.02                | 0.3        |
| (2,1886) | 1:36:A:THR:H    | 1:37:A:ASP:HA   | 10                  | 0.3      | 0.06                | 0.3        |
| (2,1353) | 1:92:A:TYR:HB3  | 1:64:A:PHE:HB3  | 10                  | 0.3      | 0.07                | 0.28       |
| (2,2820) | 1:58:A:LYS:H    | 1:60:A:VAL:HB   | 10                  | 0.3      | 0.03                | 0.31       |
| (1,128)  | 1:21:A:ILE:O    | 1:25:A:VAL:H    | 10                  | 0.27     | 0.06                | 0.29       |
| (2,1508) | 1:47:A:ALA:H    | 1:91:A:MET:HB2  | 10                  | 0.27     | 0.05                | 0.26       |
| (2,507)  | 1:19:A:ASP:HA   | 1:22:A:ASN:HB3  | 10                  | 0.26     | 0.15                | 0.2        |
| (2,941)  | 1:111:A:LEU:HA  | 1:110:A:ASP:H   | 10                  | 0.26     | 0.09                | 0.26       |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD21 | 10                  | 0.26     | 0.02                | 0.27       |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD22 | 10                  | 0.26     | 0.02                | 0.27       |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD23 | 10                  | 0.26     | 0.02                | 0.27       |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG21 | 10                  | 0.25     | 0.07                | 0.26       |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG22 | 10                  | 0.25     | 0.07                | 0.26       |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG23 | 10                  | 0.25     | 0.07                | 0.26       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,271)  | 1:50:A:PHE:HA   | 1:51:A:LEU:H    | 10                  | 0.25     | 0.02                | 0.24       |
| (2,585)  | 1:37:A:ASP:HA   | 1:38:A:VAL:H    | 10                  | 0.25     | 0.03                | 0.25       |
| (2,369)  | 1:19:A:ASP:HA   | 1:23:A:ASN:HB3  | 10                  | 0.24     | 0.05                | 0.23       |
| (2,919)  | 1:108:A:ILE:HA  | 1:110:A:ASP:HB2 | 10                  | 0.23     | 0.07                | 0.24       |
| (2,1997) | 1:63:A:THR:H    | 1:62:A:ASN:HA   | 10                  | 0.22     | 0.02                | 0.22       |
| (2,208)  | 1:79:A:GLY:HA2  | 1:76:A:SER:HA   | 10                  | 0.2      | 0.04                | 0.21       |
| (2,2657) | 1:23:A:ASN:H    | 1:23:A:ASN:HD22 | 10                  | 0.19     | 0.09                | 0.16       |
| (2,234)  | 1:49:A:VAL:HG21 | 1:35:A:ILE:HA   | 10                  | 0.19     | 0.04                | 0.2        |
| (2,234)  | 1:49:A:VAL:HG22 | 1:35:A:ILE:HA   | 10                  | 0.19     | 0.04                | 0.2        |
| (2,234)  | 1:49:A:VAL:HG23 | 1:35:A:ILE:HA   | 10                  | 0.19     | 0.04                | 0.2        |
| (2,2428) | 1:58:A:LYS:H    | 1:56:A:ASN:HA   | 10                  | 0.18     | 0.05                | 0.18       |
| (2,2991) | 1:98:A:ILE:H    | 1:99:A:GLU:HA   | 10                  | 0.18     | 0.05                | 0.18       |
| (2,25)   | 1:15:A:LYS:C    | 1:19:A:ASP:H    | 10                  | 0.17     | 0.05                | 0.16       |
| (2,87)   | 1:63:A:THR:C    | 1:67:A:LEU:H    | 10                  | 0.15     | 0.01                | 0.15       |
| (2,31)   | 1:18:A:MET:C    | 1:22:A:ASN:H    | 10                  | 0.14     | 0.02                | 0.15       |
| (1,46)   | 1:65:A:LYS:H    | 1:61:A:GLU:O    | 10                  | 0.14     | 0.03                | 0.14       |
| (2,404)  | 1:56:A:ASN:HB2  | 1:56:A:ASN:HB3  | 10                  | 0.13     | 0.0                 | 0.13       |
| (2,986)  | 1:11:A:GLU:HB3  | 1:11:A:GLU:HB2  | 10                  | 0.13     | 0.0                 | 0.13       |
| (2,415)  | 1:73:A:PHE:HB2  | 1:73:A:PHE:HB3  | 10                  | 0.12     | 0.0                 | 0.12       |
| (2,419)  | 1:73:A:PHE:HB3  | 1:73:A:PHE:HB2  | 10                  | 0.12     | 0.0                 | 0.12       |
| (2,1317) | 1:91:A:MET:HB2  | 1:48:A:LYS:HB3  | 9                   | 0.42     | 0.14                | 0.38       |
| (2,2118) | 1:112:A:HIS:H   | 1:78:A:LEU:HB3  | 9                   | 0.37     | 0.16                | 0.34       |
| (2,1092) | 1:38:A:VAL:HG21 | 1:17:A:LEU:HB3  | 9                   | 0.3      | 0.1                 | 0.32       |
| (2,1092) | 1:38:A:VAL:HG22 | 1:17:A:LEU:HB3  | 9                   | 0.3      | 0.1                 | 0.32       |
| (2,1092) | 1:38:A:VAL:HG23 | 1:17:A:LEU:HB3  | 9                   | 0.3      | 0.1                 | 0.32       |
| (2,3006) | 1:101:A:GLY:H   | 1:100:A:TYR:HA  | 9                   | 0.22     | 0.03                | 0.23       |
| (2,883)  | 1:81:A:ARG:HB3  | 1:80:A:SER:H    | 9                   | 0.19     | 0.05                | 0.21       |
| (2,1344) | 1:98:A:ILE:HG12 | 1:95:A:ASP:HB2  | 9                   | 0.19     | 0.05                | 0.17       |
| (2,2088) | 1:99:A:GLU:H    | 1:98:A:ILE:HG13 | 9                   | 0.18     | 0.04                | 0.18       |
| (2,136)  | 1:31:A:GLY:HA2  | 1:54:A:LEU:HB3  | 9                   | 0.18     | 0.04                | 0.18       |
| (2,2681) | 1:34:A:THR:H    | 1:51:A:LEU:HB2  | 9                   | 0.17     | 0.03                | 0.15       |
| (2,26)   | 1:15:A:LYS:C    | 1:19:A:ASP:N    | 9                   | 0.16     | 0.05                | 0.15       |
| (1,127)  | 1:20:A:ILE:O    | 1:24:A:LYS:H    | 9                   | 0.16     | 0.04                | 0.15       |
| (2,1688) | 1:77:A:GLU:H    | 1:73:A:PHE:HA   | 9                   | 0.15     | 0.04                | 0.15       |
| (2,1199) | 1:59:A:GLU:HB2  | 1:56:A:ASN:HD22 | 9                   | 0.15     | 0.03                | 0.14       |
| (2,457)  | 1:11:A:GLU:HA   | 1:38:A:VAL:HB   | 8                   | 0.84     | 0.28                | 0.93       |
| (2,506)  | 1:19:A:ASP:HA   | 1:18:A:MET:HB2  | 8                   | 0.53     | 0.04                | 0.53       |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG21 | 8                   | 0.34     | 0.08                | 0.36       |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG22 | 8                   | 0.34     | 0.08                | 0.36       |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG23 | 8                   | 0.34     | 0.08                | 0.36       |
| (2,938)  | 1:111:A:LEU:HA  | 1:113:A:LYS:HB3 | 8                   | 0.33     | 0.13                | 0.34       |
| (2,301)  | 1:91:A:MET:HB2  | 1:48:A:LYS:HA   | 8                   | 0.33     | 0.07                | 0.3        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,948)  | 1:111:A:LEU:HB2 | 1:112:A:HIS:HA  | 8                   | 0.24     | 0.1                 | 0.26       |
| (2,210)  | 1:78:A:LEU:HA   | 1:16:A:GLU:HB2  | 8                   | 0.24     | 0.09                | 0.24       |
| (2,2912) | 1:76:A:SER:H    | 1:77:A:GLU:HB3  | 8                   | 0.22     | 0.16                | 0.16       |
| (2,1814) | 1:14:A:LYS:H    | 1:12:A:GLN:HB2  | 8                   | 0.21     | 0.03                | 0.2        |
| (2,2096) | 1:102:A:ASN:H   | 1:101:A:GLY:HA2 | 8                   | 0.2      | 0.07                | 0.18       |
| (2,1599) | 1:62:A:ASN:H    | 1:64:A:PHE:HB3  | 8                   | 0.19     | 0.07                | 0.16       |
| (2,192)  | 1:25:A:VAL:HG21 | 1:74:A:ILE:HA   | 8                   | 0.18     | 0.05                | 0.18       |
| (2,192)  | 1:25:A:VAL:HG22 | 1:74:A:ILE:HA   | 8                   | 0.18     | 0.05                | 0.18       |
| (2,192)  | 1:25:A:VAL:HG23 | 1:74:A:ILE:HA   | 8                   | 0.18     | 0.05                | 0.18       |
| (2,19)   | 1:12:A:GLN:C    | 1:16:A:GLU:H    | 8                   | 0.18     | 0.05                | 0.18       |
| (2,2886) | 1:71:A:LYS:H    | 1:69:A:LYS:HB3  | 8                   | 0.18     | 0.05                | 0.16       |
| (2,2268) | 1:17:A:LEU:H    | 1:15:A:LYS:HB2  | 8                   | 0.18     | 0.04                | 0.18       |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG21 | 8                   | 0.17     | 0.05                | 0.16       |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG22 | 8                   | 0.17     | 0.05                | 0.16       |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG23 | 8                   | 0.17     | 0.05                | 0.16       |
| (2,20)   | 1:12:A:GLN:C    | 1:16:A:GLU:N    | 8                   | 0.16     | 0.04                | 0.15       |
| (2,510)  | 1:19:A:ASP:HA   | 1:18:A:MET:HA   | 8                   | 0.16     | 0.04                | 0.15       |
| (2,2913) | 1:77:A:GLU:H    | 1:78:A:LEU:HB2  | 8                   | 0.16     | 0.04                | 0.15       |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG21 | 8                   | 0.14     | 0.03                | 0.14       |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG22 | 8                   | 0.14     | 0.03                | 0.14       |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG23 | 8                   | 0.14     | 0.03                | 0.14       |
| (2,600)  | 1:38:A:VAL:HG21 | 1:50:A:PHE:H    | 7                   | 0.5      | 0.03                | 0.49       |
| (2,600)  | 1:38:A:VAL:HG22 | 1:50:A:PHE:H    | 7                   | 0.5      | 0.03                | 0.49       |
| (2,600)  | 1:38:A:VAL:HG23 | 1:50:A:PHE:H    | 7                   | 0.5      | 0.03                | 0.49       |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG21 | 7                   | 0.3      | 0.19                | 0.19       |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG22 | 7                   | 0.3      | 0.19                | 0.19       |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG23 | 7                   | 0.3      | 0.19                | 0.19       |
| (2,2752) | 1:46:A:GLN:HE22 | 1:46:A:GLN:HA   | 7                   | 0.28     | 0.08                | 0.28       |
| (2,215)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB3  | 7                   | 0.27     | 0.11                | 0.28       |
| (2,215)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB3  | 7                   | 0.27     | 0.11                | 0.28       |
| (2,215)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB3  | 7                   | 0.27     | 0.11                | 0.28       |
| (2,2038) | 1:76:A:SER:H    | 1:72:A:GLY:HA3  | 7                   | 0.24     | 0.08                | 0.24       |
| (2,2214) | 1:76:A:SER:H    | 1:78:A:LEU:HB2  | 7                   | 0.21     | 0.04                | 0.22       |
| (2,121)  | 1:45:A:SER:HA   | 1:88:A:PRO:HA   | 7                   | 0.21     | 0.08                | 0.19       |
| (2,2650) | 1:22:A:ASN:H    | 1:18:A:MET:HA   | 7                   | 0.2      | 0.03                | 0.19       |
| (1,150)  | 1:66:A:ALA:O    | 1:70:A:ALA:H    | 7                   | 0.19     | 0.11                | 0.15       |
| (2,1575) | 1:58:A:LYS:H    | 1:59:A:GLU:HG3  | 7                   | 0.18     | 0.12                | 0.13       |
| (2,2464) | 1:66:A:ALA:H    | 1:65:A:LYS:HG2  | 7                   | 0.16     | 0.03                | 0.17       |
| (2,120)  | 1:33:A:ILE:HA   | 1:53:A:VAL:HA   | 7                   | 0.16     | 0.02                | 0.16       |
| (2,2959) | 1:91:A:MET:H    | 1:47:A:ALA:HA   | 7                   | 0.16     | 0.05                | 0.13       |
| (2,2772) | 1:49:A:VAL:H    | 1:38:A:VAL:HG21 | 7                   | 0.15     | 0.02                | 0.15       |
| (2,2772) | 1:49:A:VAL:H    | 1:38:A:VAL:HG22 | 7                   | 0.15     | 0.02                | 0.15       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,2772) | 1:49:A:VAL:H    | 1:38:A:VAL:HG23 | 7                   | 0.15     | 0.02                | 0.15       |
| (2,785)  | 1:65:A:LYS:HD2  | 1:65:A:LYS:HA   | 7                   | 0.15     | 0.02                | 0.16       |
| (2,11)   | 1:8:A:ARG:C     | 1:12:A:GLN:H    | 7                   | 0.15     | 0.03                | 0.13       |
| (2,2856) | 1:63:A:THR:H    | 1:65:A:LYS:HG2  | 7                   | 0.14     | 0.04                | 0.13       |
| (2,93)   | 1:60:A:VAL:C    | 1:64:A:PHE:H    | 7                   | 0.14     | 0.02                | 0.13       |
| (2,94)   | 1:60:A:VAL:C    | 1:64:A:PHE:N    | 7                   | 0.13     | 0.02                | 0.12       |
| (2,216)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB2  | 6                   | 0.32     | 0.11                | 0.3        |
| (2,216)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB2  | 6                   | 0.32     | 0.11                | 0.3        |
| (2,216)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB2  | 6                   | 0.32     | 0.11                | 0.3        |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB1  | 6                   | 0.27     | 0.04                | 0.26       |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB2  | 6                   | 0.27     | 0.04                | 0.26       |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB3  | 6                   | 0.27     | 0.04                | 0.26       |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB1  | 6                   | 0.27     | 0.04                | 0.26       |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB2  | 6                   | 0.27     | 0.04                | 0.26       |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB3  | 6                   | 0.27     | 0.04                | 0.26       |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB1  | 6                   | 0.27     | 0.04                | 0.26       |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB2  | 6                   | 0.27     | 0.04                | 0.26       |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB3  | 6                   | 0.27     | 0.04                | 0.26       |
| (2,1616) | 1:66:A:ALA:H    | 1:65:A:LYS:HD2  | 6                   | 0.24     | 0.09                | 0.25       |
| (2,934)  | 1:109:A:GLN:HB2 | 1:110:A:ASP:HB2 | 6                   | 0.22     | 0.07                | 0.2        |
| (2,1389) | 1:15:A:LYS:H    | 1:16:A:GLU:HB2  | 6                   | 0.18     | 0.06                | 0.18       |
| (2,995)  | 1:13:A:MET:HB3  | 1:10:A:GLY:HA3  | 6                   | 0.16     | 0.04                | 0.15       |
| (1,116)  | 1:9:A:VAL:O     | 1:13:A:MET:H    | 6                   | 0.15     | 0.02                | 0.15       |
| (2,1617) | 1:66:A:ALA:H    | 1:69:A:LYS:HB3  | 6                   | 0.15     | 0.02                | 0.15       |
| (1,153)  | 1:63:A:THR:O    | 1:67:A:LEU:H    | 6                   | 0.14     | 0.01                | 0.14       |
| (2,175)  | 1:72:A:GLY:HA3  | 1:75:A:LYS:HB3  | 6                   | 0.14     | 0.02                | 0.14       |
| (2,848)  | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 6                   | 0.14     | 0.02                | 0.14       |
| (1,117)  | 1:10:A:GLY:O    | 1:14:A:LYS:H    | 6                   | 0.13     | 0.02                | 0.14       |
| (2,2743) | 1:45:A:SER:H    | 1:46:A:GLN:HA   | 6                   | 0.13     | 0.02                | 0.12       |
| (2,2119) | 1:113:A:LYS:H   | 1:78:A:LEU:HB3  | 5                   | 0.4      | 0.12                | 0.44       |
| (2,125)  | 1:49:A:VAL:H    | 1:92:A:TYR:HA   | 5                   | 0.23     | 0.02                | 0.23       |
| (2,960)  | 1:118:A:GLU:HA  | 1:117:A:VAL:HB  | 5                   | 0.17     | 0.06                | 0.16       |
| (2,238)  | 1:95:A:ASP:HA   | 1:50:A:PHE:HD1  | 5                   | 0.17     | 0.01                | 0.16       |
| (2,238)  | 1:95:A:ASP:HA   | 1:50:A:PHE:HD2  | 5                   | 0.17     | 0.01                | 0.16       |
| (2,1247) | 1:68:A:ASP:HB2  | 1:71:A:LYS:HG3  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,137)  | 1:48:A:LYS:O    | 1:39:A:VAL:H    | 5                   | 0.16     | 0.05                | 0.14       |
| (2,2758) | 1:47:A:ALA:H    | 1:89:A:GLU:HB3  | 5                   | 0.16     | 0.05                | 0.12       |
| (1,143)  | 1:76:A:SER:O    | 1:80:A:SER:H    | 5                   | 0.14     | 0.04                | 0.15       |
| (2,1495) | 1:46:A:GLN:H    | 1:45:A:SER:H    | 5                   | 0.14     | 0.02                | 0.14       |
| (2,2588) | 1:22:A:ASN:H    | 1:22:A:ASN:HD22 | 5                   | 0.14     | 0.04                | 0.12       |
| (1,42)   | 1:69:A:LYS:H    | 1:65:A:LYS:O    | 5                   | 0.13     | 0.02                | 0.13       |
| (1,118)  | 1:11:A:GLU:O    | 1:15:A:LYS:H    | 5                   | 0.13     | 0.02                | 0.13       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,281)  | 1:10:A:GLY:HA2  | 1:38:A:VAL:HB   | 5                   | 0.13     | 0.01                | 0.12       |
| (2,1265) | 1:71:A:LYS:HB2  | 1:75:A:LYS:HG2  | 4                   | 0.25     | 0.03                | 0.24       |
| (2,2090) | 1:99:A:GLU:H    | 1:101:A:GLY:HA2 | 4                   | 0.22     | 0.11                | 0.18       |
| (2,239)  | 1:50:A:PHE:HB3  | 1:95:A:ASP:HA   | 4                   | 0.2      | 0.06                | 0.19       |
| (2,1876) | 1:34:A:THR:H    | 1:52:A:THR:HB   | 4                   | 0.2      | 0.05                | 0.2        |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG11 | 4                   | 0.2      | 0.01                | 0.2        |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG12 | 4                   | 0.2      | 0.01                | 0.2        |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG13 | 4                   | 0.2      | 0.01                | 0.2        |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG21 | 4                   | 0.19     | 0.02                | 0.2        |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG22 | 4                   | 0.19     | 0.02                | 0.2        |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG23 | 4                   | 0.19     | 0.02                | 0.2        |
| (2,528)  | 1:22:A:ASN:HA   | 1:33:A:ILE:HB   | 4                   | 0.16     | 0.04                | 0.15       |
| (2,79)   | 1:70:A:ALA:C    | 1:74:A:ILE:H    | 4                   | 0.16     | 0.07                | 0.13       |
| (2,1002) | 1:16:A:GLU:HB2  | 1:81:A:ARG:HB3  | 4                   | 0.15     | 0.04                | 0.16       |
| (2,1313) | 1:81:A:ARG:HB3  | 1:16:A:GLU:HB2  | 4                   | 0.15     | 0.04                | 0.16       |
| (2,5)    | 1:5:A:ARG:C     | 1:9:A:VAL:H     | 4                   | 0.15     | 0.02                | 0.15       |
| (2,6)    | 1:5:A:ARG:C     | 1:9:A:VAL:N     | 4                   | 0.14     | 0.02                | 0.15       |
| (2,13)   | 1:9:A:VAL:C     | 1:13:A:MET:H    | 4                   | 0.14     | 0.03                | 0.14       |
| (2,2692) | 1:35:A:ILE:H    | 1:36:A:THR:HA   | 4                   | 0.13     | 0.01                | 0.12       |
| (1,159)  | 1:57:A:ASP:O    | 1:61:A:GLU:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (2,1095) | 1:38:A:VAL:HG21 | 1:39:A:VAL:HA   | 3                   | 0.99     | 0.02                | 0.97       |
| (2,1095) | 1:38:A:VAL:HG22 | 1:39:A:VAL:HA   | 3                   | 0.99     | 0.02                | 0.97       |
| (2,1095) | 1:38:A:VAL:HG23 | 1:39:A:VAL:HA   | 3                   | 0.99     | 0.02                | 0.97       |
| (2,1784) | 1:12:A:GLN:HE22 | 1:12:A:GLN:HA   | 3                   | 0.47     | 0.16                | 0.58       |
| (2,1832) | 1:16:A:GLU:H    | 1:12:A:GLN:HB2  | 3                   | 0.4      | 0.1                 | 0.42       |
| (2,2738) | 1:43:A:ASP:H    | 1:41:A:THR:HG1  | 3                   | 0.32     | 0.29                | 0.11       |
| (2,616)  | 1:39:A:VAL:HG21 | 1:40:A:LEU:H    | 3                   | 0.31     | 0.02                | 0.3        |
| (2,616)  | 1:39:A:VAL:HG22 | 1:40:A:LEU:H    | 3                   | 0.31     | 0.02                | 0.3        |
| (2,616)  | 1:39:A:VAL:HG23 | 1:40:A:LEU:H    | 3                   | 0.31     | 0.02                | 0.3        |
| (2,526)  | 1:22:A:ASN:HA   | 1:22:A:ASN:HD22 | 3                   | 0.29     | 0.07                | 0.25       |
| (2,1106) | 1:39:A:VAL:HG21 | 1:48:A:LYS:HB3  | 3                   | 0.23     | 0.11                | 0.19       |
| (2,1106) | 1:39:A:VAL:HG22 | 1:48:A:LYS:HB3  | 3                   | 0.23     | 0.11                | 0.19       |
| (2,1106) | 1:39:A:VAL:HG23 | 1:48:A:LYS:HB3  | 3                   | 0.23     | 0.11                | 0.19       |
| (2,1849) | 1:21:A:ILE:H    | 1:25:A:VAL:HB   | 3                   | 0.22     | 0.04                | 0.2        |
| (2,1822) | 1:15:A:LYS:H    | 1:12:A:GLN:HB2  | 3                   | 0.21     | 0.04                | 0.24       |
| (2,126)  | 1:93:A:GLU:H    | 1:50:A:PHE:HA   | 3                   | 0.19     | 0.07                | 0.17       |
| (2,1058) | 1:33:A:ILE:HB   | 1:22:A:ASN:HD22 | 3                   | 0.18     | 0.03                | 0.2        |
| (2,1216) | 1:62:A:ASN:HA   | 1:65:A:LYS:HD2  | 3                   | 0.18     | 0.04                | 0.16       |
| (2,2899) | 1:74:A:ILE:H    | 1:71:A:LYS:HB3  | 3                   | 0.18     | 0.02                | 0.18       |
| (2,437)  | 1:6:A:ALA:HB1   | 1:39:A:VAL:HG21 | 3                   | 0.17     | 0.03                | 0.19       |
| (2,437)  | 1:6:A:ALA:HB1   | 1:39:A:VAL:HG22 | 3                   | 0.17     | 0.03                | 0.19       |
| (2,437)  | 1:6:A:ALA:HB1   | 1:39:A:VAL:HG23 | 3                   | 0.17     | 0.03                | 0.19       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (2,437)  | 1:6:A:ALA:HB2   | 1:39:A:VAL:HG21  | 3                   | 0.17     | 0.03                | 0.19       |
| (2,437)  | 1:6:A:ALA:HB2   | 1:39:A:VAL:HG22  | 3                   | 0.17     | 0.03                | 0.19       |
| (2,437)  | 1:6:A:ALA:HB2   | 1:39:A:VAL:HG23  | 3                   | 0.17     | 0.03                | 0.19       |
| (2,437)  | 1:6:A:ALA:HB3   | 1:39:A:VAL:HG21  | 3                   | 0.17     | 0.03                | 0.19       |
| (2,437)  | 1:6:A:ALA:HB3   | 1:39:A:VAL:HG22  | 3                   | 0.17     | 0.03                | 0.19       |
| (2,437)  | 1:6:A:ALA:HB3   | 1:39:A:VAL:HG23  | 3                   | 0.17     | 0.03                | 0.19       |
| (2,2062) | 1:91:A:MET:H    | 1:49:A:VAL:HB    | 3                   | 0.15     | 0.03                | 0.16       |
| (2,994)  | 1:13:A:MET:HB3  | 1:38:A:VAL:HB    | 3                   | 0.15     | 0.01                | 0.15       |
| (2,12)   | 1:8:A:ARG:C     | 1:12:A:GLN:N     | 3                   | 0.15     | 0.03                | 0.16       |
| (2,17)   | 1:11:A:GLU:C    | 1:15:A:LYS:H     | 3                   | 0.14     | 0.02                | 0.13       |
| (2,1823) | 1:15:A:LYS:H    | 1:18:A:MET:HB2   | 3                   | 0.14     | 0.02                | 0.15       |
| (2,2975) | 1:96:A:GLN:H    | 1:96:A:GLN:HE22  | 3                   | 0.14     | 0.02                | 0.13       |
| (2,32)   | 1:18:A:MET:C    | 1:22:A:ASN:N     | 3                   | 0.14     | 0.02                | 0.14       |
| (1,122)  | 1:15:A:LYS:O    | 1:19:A:ASP:H     | 3                   | 0.13     | 0.02                | 0.12       |
| (2,1227) | 1:65:A:LYS:HG2  | 1:61:A:GLU:HB2   | 3                   | 0.13     | 0.02                | 0.12       |
| (2,1701) | 1:79:A:GLY:H    | 1:75:A:LYS:HB3   | 3                   | 0.13     | 0.02                | 0.12       |
| (2,29)   | 1:17:A:LEU:C    | 1:21:A:ILE:H     | 3                   | 0.12     | 0.01                | 0.13       |
| (1,119)  | 1:12:A:GLN:O    | 1:16:A:GLU:H     | 3                   | 0.12     | 0.02                | 0.12       |
| (1,39)   | 1:75:A:LYS:H    | 1:71:A:LYS:O     | 3                   | 0.12     | 0.02                | 0.11       |
| (2,1155) | 1:52:A:THR:HB   | 1:34:A:THR:HG1   | 3                   | 0.12     | 0.0                 | 0.12       |
| (2,2025) | 1:73:A:PHE:H    | 1:71:A:LYS:HB2   | 3                   | 0.11     | 0.0                 | 0.11       |
| (2,2441) | 1:60:A:VAL:H    | 1:59:A:GLU:HG2   | 2                   | 0.32     | 0.02                | 0.32       |
| (2,931)  | 1:109:A:GLN:HB2 | 1:109:A:GLN:HE22 | 2                   | 0.22     | 0.08                | 0.22       |
| (2,1031) | 1:24:A:LYS:HB2  | 1:25:A:VAL:HG11  | 2                   | 0.22     | 0.07                | 0.22       |
| (2,1031) | 1:24:A:LYS:HB2  | 1:25:A:VAL:HG12  | 2                   | 0.22     | 0.07                | 0.22       |
| (2,1031) | 1:24:A:LYS:HB2  | 1:25:A:VAL:HG13  | 2                   | 0.22     | 0.07                | 0.22       |
| (2,80)   | 1:70:A:ALA:C    | 1:74:A:ILE:N     | 2                   | 0.21     | 0.06                | 0.21       |
| (2,330)  | 1:48:A:LYS:HD3  | 1:93:A:GLU:HB2   | 2                   | 0.2      | 0.0                 | 0.2        |
| (2,582)  | 1:36:A:THR:HG21 | 1:51:A:LEU:H     | 2                   | 0.18     | 0.04                | 0.18       |
| (2,582)  | 1:36:A:THR:HG22 | 1:51:A:LEU:H     | 2                   | 0.18     | 0.04                | 0.18       |
| (2,582)  | 1:36:A:THR:HG23 | 1:51:A:LEU:H     | 2                   | 0.18     | 0.04                | 0.18       |
| (2,2124) | 1:117:A:VAL:H   | 1:117:A:VAL:HB   | 2                   | 0.18     | 0.02                | 0.18       |
| (2,270)  | 1:47:A:ALA:HA   | 1:40:A:LEU:HA    | 2                   | 0.17     | 0.01                | 0.17       |
| (2,334)  | 1:17:A:LEU:HD21 | 1:13:A:MET:HB3   | 2                   | 0.16     | 0.02                | 0.16       |
| (2,334)  | 1:17:A:LEU:HD22 | 1:13:A:MET:HB3   | 2                   | 0.16     | 0.02                | 0.16       |
| (2,334)  | 1:17:A:LEU:HD23 | 1:13:A:MET:HB3   | 2                   | 0.16     | 0.02                | 0.16       |
| (2,1093) | 1:38:A:VAL:HG21 | 1:10:A:GLY:HA3   | 2                   | 0.16     | 0.05                | 0.16       |
| (2,1093) | 1:38:A:VAL:HG22 | 1:10:A:GLY:HA3   | 2                   | 0.16     | 0.05                | 0.16       |
| (2,1093) | 1:38:A:VAL:HG23 | 1:10:A:GLY:HA3   | 2                   | 0.16     | 0.05                | 0.16       |
| (2,2804) | 1:56:A:ASN:HD22 | 1:56:A:ASN:HA    | 2                   | 0.16     | 0.02                | 0.16       |
| (2,14)   | 1:9:A:VAL:C     | 1:13:A:MET:N     | 2                   | 0.15     | 0.0                 | 0.15       |
| (2,1992) | 1:64:A:PHE:H    | 1:62:A:ASN:HB2   | 2                   | 0.14     | 0.03                | 0.14       |

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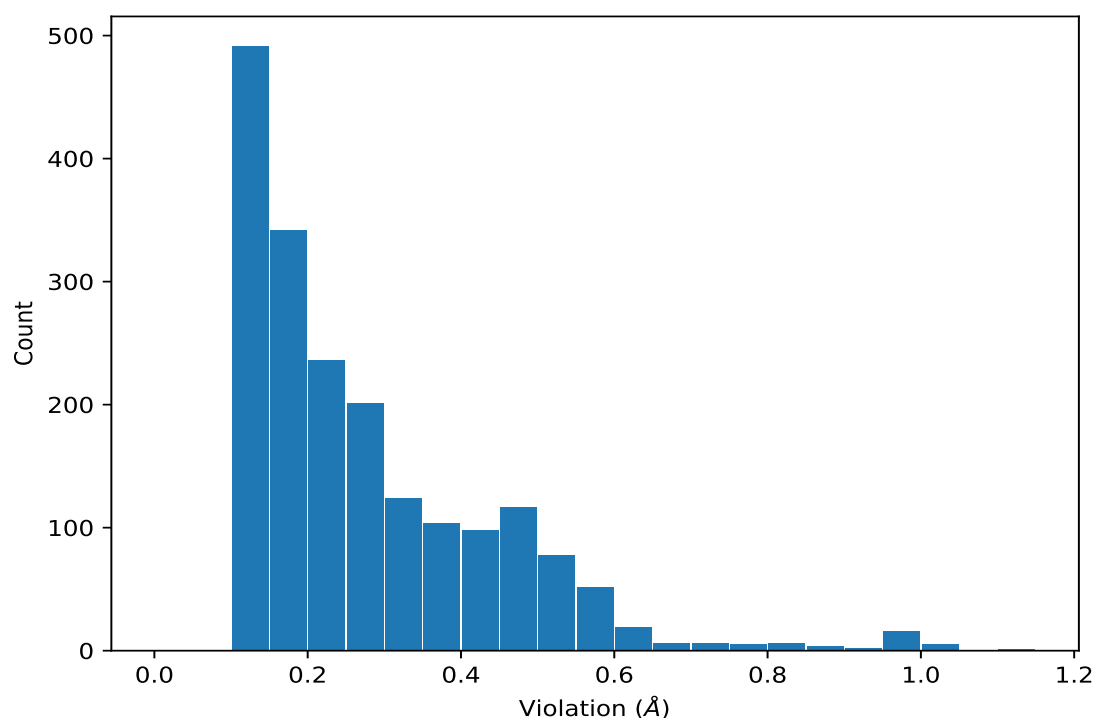
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,2960) | 1:91:A:MET:H    | 1:92:A:TYR:HA   | 2                   | 0.14     | 0.01                | 0.14       |
| (1,115)  | 1:8:A:ARG:O     | 1:12:A:GLN:H    | 2                   | 0.14     | 0.02                | 0.14       |
| (2,2737) | 1:43:A:ASP:H    | 1:45:A:SER:HB3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,114)  | 1:7:A:GLU:O     | 1:11:A:GLU:H    | 2                   | 0.13     | 0.02                | 0.13       |
| (2,917)  | 1:108:A:ILE:HA  | 1:107:A:MET:HB2 | 2                   | 0.13     | 0.02                | 0.13       |
| (2,1628) | 1:68:A:ASP:H    | 1:69:A:LYS:HB3  | 2                   | 0.13     | 0.02                | 0.13       |
| (2,261)  | 1:94:A:TYR:HE1  | 1:53:A:VAL:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (2,261)  | 1:94:A:TYR:HE2  | 1:53:A:VAL:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (2,760)  | 1:62:A:ASN:HB2  | 1:59:A:GLU:HA   | 2                   | 0.12     | 0.01                | 0.12       |
| (2,2014) | 1:68:A:ASP:H    | 1:65:A:LYS:HB2  | 2                   | 0.12     | 0.02                | 0.12       |
| (2,2054) | 1:89:A:GLU:H    | 1:46:A:GLN:HG2  | 2                   | 0.12     | 0.01                | 0.12       |
| (2,2819) | 1:58:A:LYS:H    | 1:59:A:GLU:HB2  | 2                   | 0.12     | 0.02                | 0.12       |
| (2,737)  | 1:59:A:GLU:HG3  | 1:56:A:ASN:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (2,2382) | 1:48:A:LYS:H    | 1:48:A:LYS:HD3  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,156)  | 1:60:A:VAL:O    | 1:64:A:PHE:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (2,67)   | 1:76:A:SER:C    | 1:80:A:SER:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,51)   | 1:60:A:VAL:H    | 1:56:A:ASN:O    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,139)  | 1:39:A:VAL:O    | 1:48:A:LYS:H    | 2                   | 0.11     | 0.01                | 0.11       |
| (2,70)   | 1:75:A:LYS:C    | 1:79:A:GLY:N    | 2                   | 0.11     | 0.01                | 0.11       |
| (2,1170) | 1:53:A:VAL:HB   | 1:51:A:LEU:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,2338) | 1:35:A:ILE:H    | 1:36:A:THR:HG21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,2338) | 1:35:A:ILE:H    | 1:36:A:THR:HG22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,2338) | 1:35:A:ILE:H    | 1:36:A:THR:HG23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,2398) | 1:49:A:VAL:H    | 1:50:A:PHE:HD1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,2398) | 1:49:A:VAL:H    | 1:50:A:PHE:HD2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,254)  | 1:22:A:ASN:HD22 | 1:33:A:ILE:HB   | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,88)   | 1:63:A:THR:C    | 1:67:A:LEU:N    | 2                   | 0.1      | 0.0                 | 0.1        |

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

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

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

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



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

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

| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (2,457)  | 1:11:A:GLU:HA   | 1:38:A:VAL:HB  | 3        | 1.12          |
| (2,1095) | 1:38:A:VAL:HG21 | 1:39:A:VAL:HA  | 5        | 1.02          |
| (2,1095) | 1:38:A:VAL:HG22 | 1:39:A:VAL:HA  | 5        | 1.02          |
| (2,1095) | 1:38:A:VAL:HG23 | 1:39:A:VAL:HA  | 5        | 1.02          |
| (2,3028) | 1:113:A:LYS:H   | 1:113:A:LYS:HA | 10       | 1.01          |
| (2,3028) | 1:113:A:LYS:H   | 1:113:A:LYS:HA | 8        | 1.0           |
| (2,3028) | 1:113:A:LYS:H   | 1:113:A:LYS:HA | 3        | 0.99          |
| (2,3028) | 1:113:A:LYS:H   | 1:113:A:LYS:HA | 4        | 0.99          |
| (2,457)  | 1:11:A:GLU:HA   | 1:38:A:VAL:HB  | 2        | 0.99          |
| (2,3028) | 1:113:A:LYS:H   | 1:113:A:LYS:HA | 1        | 0.98          |
| (2,3028) | 1:113:A:LYS:H   | 1:113:A:LYS:HA | 6        | 0.98          |
| (2,3028) | 1:113:A:LYS:H   | 1:113:A:LYS:HA | 2        | 0.97          |
| (2,3028) | 1:113:A:LYS:H   | 1:113:A:LYS:HA | 5        | 0.97          |
| (2,3028) | 1:113:A:LYS:H   | 1:113:A:LYS:HA | 7        | 0.97          |
| (2,3028) | 1:113:A:LYS:H   | 1:113:A:LYS:HA | 9        | 0.97          |
| (2,1095) | 1:38:A:VAL:HG21 | 1:39:A:VAL:HA  | 8        | 0.97          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1095) | 1:38:A:VAL:HG22 | 1:39:A:VAL:HA   | 8        | 0.97          |
| (2,1095) | 1:38:A:VAL:HG23 | 1:39:A:VAL:HA   | 8        | 0.97          |
| (2,1095) | 1:38:A:VAL:HG21 | 1:39:A:VAL:HA   | 10       | 0.97          |
| (2,1095) | 1:38:A:VAL:HG22 | 1:39:A:VAL:HA   | 10       | 0.97          |
| (2,1095) | 1:38:A:VAL:HG23 | 1:39:A:VAL:HA   | 10       | 0.97          |
| (2,457)  | 1:11:A:GLU:HA   | 1:38:A:VAL:HB   | 1        | 0.95          |
| (2,457)  | 1:11:A:GLU:HA   | 1:38:A:VAL:HB   | 9        | 0.94          |
| (2,457)  | 1:11:A:GLU:HA   | 1:38:A:VAL:HB   | 4        | 0.92          |
| (2,950)  | 1:111:A:LEU:HB2 | 1:110:A:ASP:HB2 | 1        | 0.89          |
| (2,457)  | 1:11:A:GLU:HA   | 1:38:A:VAL:HB   | 6        | 0.88          |
| (2,1984) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 1        | 0.86          |
| (2,1984) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 7        | 0.85          |
| (2,1984) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 2        | 0.82          |
| (2,1984) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 5        | 0.81          |
| (2,1984) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 9        | 0.81          |
| (2,1984) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 6        | 0.8           |
| (2,1984) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 10       | 0.8           |
| (2,457)  | 1:11:A:GLU:HA   | 1:38:A:VAL:HB   | 7        | 0.8           |
| (2,1984) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 4        | 0.79          |
| (2,1984) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 3        | 0.78          |
| (2,1984) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 8        | 0.78          |
| (2,950)  | 1:111:A:LEU:HB2 | 1:110:A:ASP:HB2 | 2        | 0.78          |
| (2,950)  | 1:111:A:LEU:HB2 | 1:110:A:ASP:HB2 | 8        | 0.75          |
| (2,2738) | 1:43:A:ASP:H    | 1:41:A:THR:HG1  | 8        | 0.73          |
| (2,950)  | 1:111:A:LEU:HB2 | 1:110:A:ASP:HB2 | 3        | 0.72          |
| (2,1105) | 1:39:A:VAL:HG21 | 1:37:A:ASP:HB2  | 9        | 0.71          |
| (2,1105) | 1:39:A:VAL:HG22 | 1:37:A:ASP:HB2  | 9        | 0.71          |
| (2,1105) | 1:39:A:VAL:HG23 | 1:37:A:ASP:HB2  | 9        | 0.71          |
| (2,1317) | 1:91:A:MET:HB2  | 1:48:A:LYS:HB3  | 3        | 0.7           |
| (2,2869) | 1:68:A:ASP:H    | 1:92:A:TYR:HB3  | 9        | 0.68          |
| (2,1792) | 1:3:A:SER:H     | 1:3:A:SER:HA    | 1        | 0.68          |
| (2,1792) | 1:3:A:SER:H     | 1:3:A:SER:HA    | 9        | 0.68          |
| (2,2869) | 1:68:A:ASP:H    | 1:92:A:TYR:HB3  | 2        | 0.65          |
| (2,1792) | 1:3:A:SER:H     | 1:3:A:SER:HA    | 6        | 0.65          |
| (2,1792) | 1:3:A:SER:H     | 1:3:A:SER:HA    | 7        | 0.65          |
| (2,2912) | 1:76:A:SER:H    | 1:77:A:GLU:HB3  | 10       | 0.64          |
| (2,1792) | 1:3:A:SER:H     | 1:3:A:SER:HA    | 2        | 0.64          |
| (2,507)  | 1:19:A:ASP:HA   | 1:22:A:ASN:HB3  | 2        | 0.64          |
| (2,2247) | 1:11:A:GLU:H    | 1:12:A:GLN:HA   | 4        | 0.63          |
| (2,1792) | 1:3:A:SER:H     | 1:3:A:SER:HA    | 5        | 0.63          |
| (2,1317) | 1:91:A:MET:HB2  | 1:48:A:LYS:HB3  | 8        | 0.63          |
| (2,2869) | 1:68:A:ASP:H    | 1:92:A:TYR:HB3  | 6        | 0.62          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2247) | 1:11:A:GLU:H    | 1:12:A:GLN:HA   | 7        | 0.62          |
| (2,2877) | 1:69:A:LYS:H    | 1:65:A:LYS:HB2  | 8        | 0.61          |
| (2,1792) | 1:3:A:SER:H     | 1:3:A:SER:HA    | 4        | 0.61          |
| (2,2869) | 1:68:A:ASP:H    | 1:92:A:TYR:HB3  | 4        | 0.6           |
| (2,2247) | 1:11:A:GLU:H    | 1:12:A:GLN:HA   | 3        | 0.6           |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG21 | 10       | 0.6           |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG22 | 10       | 0.6           |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG23 | 10       | 0.6           |
| (2,1792) | 1:3:A:SER:H     | 1:3:A:SER:HA    | 10       | 0.6           |
| (2,604)  | 1:38:A:VAL:HG21 | 1:47:A:ALA:HA   | 3        | 0.6           |
| (2,604)  | 1:38:A:VAL:HG22 | 1:47:A:ALA:HA   | 3        | 0.6           |
| (2,604)  | 1:38:A:VAL:HG23 | 1:47:A:ALA:HA   | 3        | 0.6           |
| (2,2859) | 1:65:A:LYS:H    | 1:61:A:GLU:HB2  | 7        | 0.59          |
| (2,2118) | 1:112:A:HIS:H   | 1:78:A:LEU:HB3  | 2        | 0.59          |
| (2,1792) | 1:3:A:SER:H     | 1:3:A:SER:HA    | 3        | 0.59          |
| (2,1792) | 1:3:A:SER:H     | 1:3:A:SER:HA    | 8        | 0.59          |
| (2,506)  | 1:19:A:ASP:HA   | 1:18:A:MET:HB2  | 7        | 0.59          |
| (2,506)  | 1:19:A:ASP:HA   | 1:18:A:MET:HB2  | 9        | 0.59          |
| (2,2247) | 1:11:A:GLU:H    | 1:12:A:GLN:HA   | 1        | 0.58          |
| (2,2247) | 1:11:A:GLU:H    | 1:12:A:GLN:HA   | 2        | 0.58          |
| (2,2247) | 1:11:A:GLU:H    | 1:12:A:GLN:HA   | 9        | 0.58          |
| (2,1784) | 1:12:A:GLN:HE22 | 1:12:A:GLN:HA   | 6        | 0.58          |
| (2,1784) | 1:12:A:GLN:HE22 | 1:12:A:GLN:HA   | 9        | 0.58          |
| (2,1098) | 1:38:A:VAL:HG21 | 1:17:A:LEU:H    | 7        | 0.58          |
| (2,1098) | 1:38:A:VAL:HG22 | 1:17:A:LEU:H    | 7        | 0.58          |
| (2,1098) | 1:38:A:VAL:HG23 | 1:17:A:LEU:H    | 7        | 0.58          |
| (2,1096) | 1:38:A:VAL:HG21 | 1:37:A:ASP:HA   | 3        | 0.58          |
| (2,1096) | 1:38:A:VAL:HG22 | 1:37:A:ASP:HA   | 3        | 0.58          |
| (2,1096) | 1:38:A:VAL:HG23 | 1:37:A:ASP:HA   | 3        | 0.58          |
| (2,2118) | 1:112:A:HIS:H   | 1:78:A:LEU:HB3  | 1        | 0.57          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD21 | 2        | 0.57          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD22 | 2        | 0.57          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD23 | 2        | 0.57          |
| (2,932)  | 1:109:A:GLN:HB2 | 1:107:A:MET:HA  | 9        | 0.57          |
| (2,2869) | 1:68:A:ASP:H    | 1:92:A:TYR:HB3  | 8        | 0.56          |
| (2,2859) | 1:65:A:LYS:H    | 1:61:A:GLU:HB2  | 2        | 0.56          |
| (2,2859) | 1:65:A:LYS:H    | 1:61:A:GLU:HB2  | 5        | 0.56          |
| (2,2859) | 1:65:A:LYS:H    | 1:61:A:GLU:HB2  | 6        | 0.56          |
| (2,2247) | 1:11:A:GLU:H    | 1:12:A:GLN:HA   | 5        | 0.56          |
| (2,2247) | 1:11:A:GLU:H    | 1:12:A:GLN:HA   | 6        | 0.56          |
| (2,2247) | 1:11:A:GLU:H    | 1:12:A:GLN:HA   | 8        | 0.56          |
| (2,1105) | 1:39:A:VAL:HG21 | 1:37:A:ASP:HB2  | 3        | 0.56          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1105) | 1:39:A:VAL:HG22 | 1:37:A:ASP:HB2  | 3        | 0.56          |
| (2,1105) | 1:39:A:VAL:HG23 | 1:37:A:ASP:HB2  | 3        | 0.56          |
| (2,1102) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HA   | 10       | 0.56          |
| (2,1102) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HA   | 10       | 0.56          |
| (2,1102) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HA   | 10       | 0.56          |
| (2,1098) | 1:38:A:VAL:HG21 | 1:17:A:LEU:H    | 4        | 0.56          |
| (2,1098) | 1:38:A:VAL:HG22 | 1:17:A:LEU:H    | 4        | 0.56          |
| (2,1098) | 1:38:A:VAL:HG23 | 1:17:A:LEU:H    | 4        | 0.56          |
| (2,600)  | 1:38:A:VAL:HG21 | 1:50:A:PHE:H    | 7        | 0.56          |
| (2,600)  | 1:38:A:VAL:HG22 | 1:50:A:PHE:H    | 7        | 0.56          |
| (2,600)  | 1:38:A:VAL:HG23 | 1:50:A:PHE:H    | 7        | 0.56          |
| (2,2869) | 1:68:A:ASP:H    | 1:92:A:TYR:HB3  | 3        | 0.55          |
| (2,2859) | 1:65:A:LYS:H    | 1:61:A:GLU:HB2  | 9        | 0.55          |
| (2,2247) | 1:11:A:GLU:H    | 1:12:A:GLN:HA   | 10       | 0.55          |
| (2,2119) | 1:113:A:LYS:H   | 1:78:A:LEU:HB3  | 10       | 0.55          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD21 | 3        | 0.55          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD22 | 3        | 0.55          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD23 | 3        | 0.55          |
| (2,1096) | 1:38:A:VAL:HG21 | 1:37:A:ASP:HA   | 4        | 0.55          |
| (2,1096) | 1:38:A:VAL:HG22 | 1:37:A:ASP:HA   | 4        | 0.55          |
| (2,1096) | 1:38:A:VAL:HG23 | 1:37:A:ASP:HA   | 4        | 0.55          |
| (2,506)  | 1:19:A:ASP:HA   | 1:18:A:MET:HB2  | 6        | 0.55          |
| (2,2859) | 1:65:A:LYS:H    | 1:61:A:GLU:HB2  | 1        | 0.54          |
| (2,2859) | 1:65:A:LYS:H    | 1:61:A:GLU:HB2  | 3        | 0.54          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD21 | 8        | 0.54          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD22 | 8        | 0.54          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD23 | 8        | 0.54          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD21 | 10       | 0.54          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD22 | 10       | 0.54          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD23 | 10       | 0.54          |
| (2,1098) | 1:38:A:VAL:HG21 | 1:17:A:LEU:H    | 2        | 0.54          |
| (2,1098) | 1:38:A:VAL:HG22 | 1:17:A:LEU:H    | 2        | 0.54          |
| (2,1098) | 1:38:A:VAL:HG23 | 1:17:A:LEU:H    | 2        | 0.54          |
| (2,938)  | 1:111:A:LEU:HA  | 1:113:A:LYS:HB3 | 6        | 0.54          |
| (2,601)  | 1:38:A:VAL:HG21 | 1:48:A:LYS:H    | 2        | 0.54          |
| (2,601)  | 1:38:A:VAL:HG22 | 1:48:A:LYS:H    | 2        | 0.54          |
| (2,601)  | 1:38:A:VAL:HG23 | 1:48:A:LYS:H    | 2        | 0.54          |
| (2,601)  | 1:38:A:VAL:HG21 | 1:48:A:LYS:H    | 7        | 0.54          |
| (2,601)  | 1:38:A:VAL:HG22 | 1:48:A:LYS:H    | 7        | 0.54          |
| (2,601)  | 1:38:A:VAL:HG23 | 1:48:A:LYS:H    | 7        | 0.54          |
| (2,600)  | 1:38:A:VAL:HG21 | 1:50:A:PHE:H    | 9        | 0.54          |
| (2,600)  | 1:38:A:VAL:HG22 | 1:50:A:PHE:H    | 9        | 0.54          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,600)  | 1:38:A:VAL:HG23 | 1:50:A:PHE:H    | 9        | 0.54          |
| (2,506)  | 1:19:A:ASP:HA   | 1:18:A:MET:HB2  | 5        | 0.54          |
| (2,2859) | 1:65:A:LYS:H    | 1:61:A:GLU:HB2  | 8        | 0.53          |
| (2,2859) | 1:65:A:LYS:H    | 1:61:A:GLU:HB2  | 10       | 0.53          |
| (2,1102) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HA   | 8        | 0.53          |
| (2,1102) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HA   | 8        | 0.53          |
| (2,1102) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HA   | 8        | 0.53          |
| (2,932)  | 1:109:A:GLN:HB2 | 1:107:A:MET:HA  | 6        | 0.53          |
| (2,2877) | 1:69:A:LYS:H    | 1:65:A:LYS:HB2  | 4        | 0.52          |
| (2,2842) | 1:61:A:GLU:H    | 1:59:A:GLU:HB2  | 4        | 0.52          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD21 | 7        | 0.52          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD22 | 7        | 0.52          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD23 | 7        | 0.52          |
| (2,1797) | 1:9:A:VAL:H     | 1:9:A:VAL:HA    | 4        | 0.52          |
| (2,1105) | 1:39:A:VAL:HG21 | 1:37:A:ASP:HB2  | 1        | 0.52          |
| (2,1105) | 1:39:A:VAL:HG22 | 1:37:A:ASP:HB2  | 1        | 0.52          |
| (2,1105) | 1:39:A:VAL:HG23 | 1:37:A:ASP:HB2  | 1        | 0.52          |
| (2,1098) | 1:38:A:VAL:HG21 | 1:17:A:LEU:H    | 6        | 0.52          |
| (2,1098) | 1:38:A:VAL:HG22 | 1:17:A:LEU:H    | 6        | 0.52          |
| (2,1098) | 1:38:A:VAL:HG23 | 1:17:A:LEU:H    | 6        | 0.52          |
| (2,600)  | 1:38:A:VAL:HG21 | 1:50:A:PHE:H    | 6        | 0.52          |
| (2,600)  | 1:38:A:VAL:HG22 | 1:50:A:PHE:H    | 6        | 0.52          |
| (2,600)  | 1:38:A:VAL:HG23 | 1:50:A:PHE:H    | 6        | 0.52          |
| (2,506)  | 1:19:A:ASP:HA   | 1:18:A:MET:HB2  | 2        | 0.52          |
| (2,2877) | 1:69:A:LYS:H    | 1:65:A:LYS:HB2  | 1        | 0.51          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB1  | 5        | 0.51          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB2  | 5        | 0.51          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB3  | 5        | 0.51          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD21 | 5        | 0.51          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD22 | 5        | 0.51          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD23 | 5        | 0.51          |
| (2,1765) | 1:109:A:GLN:H   | 1:110:A:ASP:HB3 | 5        | 0.51          |
| (2,1765) | 1:109:A:GLN:H   | 1:110:A:ASP:HB3 | 7        | 0.51          |
| (2,1098) | 1:38:A:VAL:HG21 | 1:17:A:LEU:H    | 8        | 0.51          |
| (2,1098) | 1:38:A:VAL:HG22 | 1:17:A:LEU:H    | 8        | 0.51          |
| (2,1098) | 1:38:A:VAL:HG23 | 1:17:A:LEU:H    | 8        | 0.51          |
| (2,601)  | 1:38:A:VAL:HG21 | 1:48:A:LYS:H    | 4        | 0.51          |
| (2,601)  | 1:38:A:VAL:HG22 | 1:48:A:LYS:H    | 4        | 0.51          |
| (2,601)  | 1:38:A:VAL:HG23 | 1:48:A:LYS:H    | 4        | 0.51          |
| (2,601)  | 1:38:A:VAL:HG21 | 1:48:A:LYS:H    | 6        | 0.51          |
| (2,601)  | 1:38:A:VAL:HG22 | 1:48:A:LYS:H    | 6        | 0.51          |
| (2,601)  | 1:38:A:VAL:HG23 | 1:48:A:LYS:H    | 6        | 0.51          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2877) | 1:69:A:LYS:H    | 1:65:A:LYS:HB2  | 10       | 0.5           |
| (2,2118) | 1:112:A:HIS:H   | 1:78:A:LEU:HB3  | 9        | 0.5           |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB1  | 2        | 0.5           |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB2  | 2        | 0.5           |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB3  | 2        | 0.5           |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB1  | 9        | 0.5           |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB2  | 9        | 0.5           |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB3  | 9        | 0.5           |
| (2,1832) | 1:16:A:GLU:H    | 1:12:A:GLN:HB2  | 3        | 0.5           |
| (2,1797) | 1:9:A:VAL:H     | 1:9:A:VAL:HA    | 3        | 0.5           |
| (2,1797) | 1:9:A:VAL:H     | 1:9:A:VAL:HA    | 10       | 0.5           |
| (2,1102) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HA   | 5        | 0.5           |
| (2,1102) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HA   | 5        | 0.5           |
| (2,1102) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HA   | 5        | 0.5           |
| (2,506)  | 1:19:A:ASP:HA   | 1:18:A:MET:HB2  | 1        | 0.5           |
| (2,506)  | 1:19:A:ASP:HA   | 1:18:A:MET:HB2  | 4        | 0.5           |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB1  | 4        | 0.49          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB2  | 4        | 0.49          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB3  | 4        | 0.49          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD21 | 6        | 0.49          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD22 | 6        | 0.49          |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD23 | 6        | 0.49          |
| (2,1797) | 1:9:A:VAL:H     | 1:9:A:VAL:HA    | 1        | 0.49          |
| (2,1797) | 1:9:A:VAL:H     | 1:9:A:VAL:HA    | 5        | 0.49          |
| (2,1797) | 1:9:A:VAL:H     | 1:9:A:VAL:HA    | 8        | 0.49          |
| (2,1191) | 1:57:A:ASP:HB2  | 1:56:A:ASN:HB3  | 8        | 0.49          |
| (2,1143) | 1:50:A:PHE:HB3  | 1:37:A:ASP:HB3  | 3        | 0.49          |
| (2,1102) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HA   | 9        | 0.49          |
| (2,1102) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HA   | 9        | 0.49          |
| (2,1102) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HA   | 9        | 0.49          |
| (2,1096) | 1:38:A:VAL:HG21 | 1:37:A:ASP:HA   | 10       | 0.49          |
| (2,1096) | 1:38:A:VAL:HG22 | 1:37:A:ASP:HA   | 10       | 0.49          |
| (2,1096) | 1:38:A:VAL:HG23 | 1:37:A:ASP:HA   | 10       | 0.49          |
| (2,604)  | 1:38:A:VAL:HG21 | 1:47:A:ALA:HA   | 2        | 0.49          |
| (2,604)  | 1:38:A:VAL:HG22 | 1:47:A:ALA:HA   | 2        | 0.49          |
| (2,604)  | 1:38:A:VAL:HG23 | 1:47:A:ALA:HA   | 2        | 0.49          |
| (2,601)  | 1:38:A:VAL:HG21 | 1:48:A:LYS:H    | 3        | 0.49          |
| (2,601)  | 1:38:A:VAL:HG22 | 1:48:A:LYS:H    | 3        | 0.49          |
| (2,601)  | 1:38:A:VAL:HG23 | 1:48:A:LYS:H    | 3        | 0.49          |
| (2,600)  | 1:38:A:VAL:HG21 | 1:50:A:PHE:H    | 1        | 0.49          |
| (2,600)  | 1:38:A:VAL:HG22 | 1:50:A:PHE:H    | 1        | 0.49          |
| (2,600)  | 1:38:A:VAL:HG23 | 1:50:A:PHE:H    | 1        | 0.49          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2928) | 1:79:A:GLY:H    | 1:75:A:LYS:HB2  | 3        | 0.48          |
| (2,2881) | 1:70:A:ALA:H    | 1:71:A:LYS:HB3  | 6        | 0.48          |
| (2,2877) | 1:69:A:LYS:H    | 1:65:A:LYS:HB2  | 7        | 0.48          |
| (2,2869) | 1:68:A:ASP:H    | 1:92:A:TYR:HB3  | 10       | 0.48          |
| (2,2119) | 1:113:A:LYS:H   | 1:78:A:LEU:HB3  | 3        | 0.48          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG21 | 5        | 0.48          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG22 | 5        | 0.48          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG23 | 5        | 0.48          |
| (2,1797) | 1:9:A:VAL:H     | 1:9:A:VAL:HA    | 2        | 0.48          |
| (2,1096) | 1:38:A:VAL:HG21 | 1:37:A:ASP:HA   | 8        | 0.48          |
| (2,1096) | 1:38:A:VAL:HG22 | 1:37:A:ASP:HA   | 8        | 0.48          |
| (2,1096) | 1:38:A:VAL:HG23 | 1:37:A:ASP:HA   | 8        | 0.48          |
| (2,604)  | 1:38:A:VAL:HG21 | 1:47:A:ALA:HA   | 4        | 0.48          |
| (2,604)  | 1:38:A:VAL:HG22 | 1:47:A:ALA:HA   | 4        | 0.48          |
| (2,604)  | 1:38:A:VAL:HG23 | 1:47:A:ALA:HA   | 4        | 0.48          |
| (2,600)  | 1:38:A:VAL:HG21 | 1:50:A:PHE:H    | 2        | 0.48          |
| (2,600)  | 1:38:A:VAL:HG22 | 1:50:A:PHE:H    | 2        | 0.48          |
| (2,600)  | 1:38:A:VAL:HG23 | 1:50:A:PHE:H    | 2        | 0.48          |
| (2,600)  | 1:38:A:VAL:HG21 | 1:50:A:PHE:H    | 3        | 0.48          |
| (2,600)  | 1:38:A:VAL:HG22 | 1:50:A:PHE:H    | 3        | 0.48          |
| (2,600)  | 1:38:A:VAL:HG23 | 1:50:A:PHE:H    | 3        | 0.48          |
| (2,506)  | 1:19:A:ASP:HA   | 1:18:A:MET:HB2  | 3        | 0.48          |
| (2,216)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB2  | 10       | 0.48          |
| (2,216)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB2  | 10       | 0.48          |
| (2,216)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB2  | 10       | 0.48          |
| (2,2881) | 1:70:A:ALA:H    | 1:71:A:LYS:HB3  | 9        | 0.47          |
| (2,2877) | 1:69:A:LYS:H    | 1:65:A:LYS:HB2  | 6        | 0.47          |
| (2,2859) | 1:65:A:LYS:H    | 1:61:A:GLU:HB2  | 4        | 0.47          |
| (2,2842) | 1:61:A:GLU:H    | 1:59:A:GLU:HB2  | 9        | 0.47          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB1  | 6        | 0.47          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB2  | 6        | 0.47          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB3  | 6        | 0.47          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG21 | 8        | 0.47          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG22 | 8        | 0.47          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG23 | 8        | 0.47          |
| (2,1797) | 1:9:A:VAL:H     | 1:9:A:VAL:HA    | 6        | 0.47          |
| (2,1797) | 1:9:A:VAL:H     | 1:9:A:VAL:HA    | 7        | 0.47          |
| (2,1797) | 1:9:A:VAL:H     | 1:9:A:VAL:HA    | 9        | 0.47          |
| (2,1765) | 1:109:A:GLN:H   | 1:110:A:ASP:HB3 | 8        | 0.47          |
| (2,1575) | 1:58:A:LYS:H    | 1:59:A:GLU:HG3  | 7        | 0.47          |
| (2,1096) | 1:38:A:VAL:HG21 | 1:37:A:ASP:HA   | 2        | 0.47          |
| (2,1096) | 1:38:A:VAL:HG22 | 1:37:A:ASP:HA   | 2        | 0.47          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1096) | 1:38:A:VAL:HG23 | 1:37:A:ASP:HA   | 2        | 0.47          |
| (2,938)  | 1:111:A:LEU:HA  | 1:113:A:LYS:HB3 | 1        | 0.47          |
| (2,2869) | 1:68:A:ASP:H    | 1:92:A:TYR:HB3  | 1        | 0.46          |
| (2,2842) | 1:61:A:GLU:H    | 1:59:A:GLU:HB2  | 2        | 0.46          |
| (2,2842) | 1:61:A:GLU:H    | 1:59:A:GLU:HB2  | 3        | 0.46          |
| (2,2842) | 1:61:A:GLU:H    | 1:59:A:GLU:HB2  | 10       | 0.46          |
| (2,2831) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 1        | 0.46          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB1  | 8        | 0.46          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB2  | 8        | 0.46          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB3  | 8        | 0.46          |
| (2,1098) | 1:38:A:VAL:HG21 | 1:17:A:LEU:H    | 10       | 0.46          |
| (2,1098) | 1:38:A:VAL:HG22 | 1:17:A:LEU:H    | 10       | 0.46          |
| (2,1098) | 1:38:A:VAL:HG23 | 1:17:A:LEU:H    | 10       | 0.46          |
| (2,1096) | 1:38:A:VAL:HG21 | 1:37:A:ASP:HA   | 7        | 0.46          |
| (2,1096) | 1:38:A:VAL:HG22 | 1:37:A:ASP:HA   | 7        | 0.46          |
| (2,1096) | 1:38:A:VAL:HG23 | 1:37:A:ASP:HA   | 7        | 0.46          |
| (2,950)  | 1:111:A:LEU:HB2 | 1:110:A:ASP:HB2 | 5        | 0.46          |
| (2,600)  | 1:38:A:VAL:HG21 | 1:50:A:PHE:H    | 4        | 0.46          |
| (2,600)  | 1:38:A:VAL:HG22 | 1:50:A:PHE:H    | 4        | 0.46          |
| (2,600)  | 1:38:A:VAL:HG23 | 1:50:A:PHE:H    | 4        | 0.46          |
| (2,301)  | 1:91:A:MET:HB2  | 1:48:A:LYS:HA   | 3        | 0.46          |
| (1,150)  | 1:66:A:ALA:O    | 1:70:A:ALA:H    | 7        | 0.46          |
| (2,2877) | 1:69:A:LYS:H    | 1:65:A:LYS:HB2  | 9        | 0.45          |
| (2,2842) | 1:61:A:GLU:H    | 1:59:A:GLU:HB2  | 5        | 0.45          |
| (2,2842) | 1:61:A:GLU:H    | 1:59:A:GLU:HB2  | 8        | 0.45          |
| (2,2831) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 7        | 0.45          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB1  | 1        | 0.45          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB2  | 1        | 0.45          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB3  | 1        | 0.45          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB1  | 3        | 0.45          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB2  | 3        | 0.45          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB3  | 3        | 0.45          |
| (2,1576) | 1:58:A:LYS:H    | 1:61:A:GLU:HB2  | 2        | 0.45          |
| (2,1105) | 1:39:A:VAL:HG21 | 1:37:A:ASP:HB2  | 8        | 0.45          |
| (2,1105) | 1:39:A:VAL:HG22 | 1:37:A:ASP:HB2  | 8        | 0.45          |
| (2,1105) | 1:39:A:VAL:HG23 | 1:37:A:ASP:HB2  | 8        | 0.45          |
| (2,1105) | 1:39:A:VAL:HG21 | 1:37:A:ASP:HB2  | 10       | 0.45          |
| (2,1105) | 1:39:A:VAL:HG22 | 1:37:A:ASP:HB2  | 10       | 0.45          |
| (2,1105) | 1:39:A:VAL:HG23 | 1:37:A:ASP:HB2  | 10       | 0.45          |
| (2,1098) | 1:38:A:VAL:HG21 | 1:17:A:LEU:H    | 3        | 0.45          |
| (2,1098) | 1:38:A:VAL:HG22 | 1:17:A:LEU:H    | 3        | 0.45          |
| (2,1098) | 1:38:A:VAL:HG23 | 1:17:A:LEU:H    | 3        | 0.45          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1092) | 1:38:A:VAL:HG21 | 1:17:A:LEU:HB3  | 2        | 0.45          |
| (2,1092) | 1:38:A:VAL:HG22 | 1:17:A:LEU:HB3  | 2        | 0.45          |
| (2,1092) | 1:38:A:VAL:HG23 | 1:17:A:LEU:HB3  | 2        | 0.45          |
| (2,950)  | 1:111:A:LEU:HB2 | 1:110:A:ASP:HB2 | 10       | 0.45          |
| (2,216)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB2  | 6        | 0.45          |
| (2,216)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB2  | 6        | 0.45          |
| (2,216)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB2  | 6        | 0.45          |
| (2,2842) | 1:61:A:GLU:H    | 1:59:A:GLU:HB2  | 1        | 0.44          |
| (2,2119) | 1:113:A:LYS:H   | 1:78:A:LEU:HB3  | 4        | 0.44          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB1  | 7        | 0.44          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB2  | 7        | 0.44          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB3  | 7        | 0.44          |
| (2,1317) | 1:91:A:MET:HB2  | 1:48:A:LYS:HB3  | 7        | 0.44          |
| (2,1105) | 1:39:A:VAL:HG21 | 1:37:A:ASP:HB2  | 4        | 0.44          |
| (2,1105) | 1:39:A:VAL:HG22 | 1:37:A:ASP:HB2  | 4        | 0.44          |
| (2,1105) | 1:39:A:VAL:HG23 | 1:37:A:ASP:HB2  | 4        | 0.44          |
| (2,950)  | 1:111:A:LEU:HB2 | 1:110:A:ASP:HB2 | 4        | 0.44          |
| (2,2842) | 1:61:A:GLU:H    | 1:59:A:GLU:HB2  | 6        | 0.43          |
| (2,2118) | 1:112:A:HIS:H   | 1:78:A:LEU:HB3  | 6        | 0.43          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB1  | 10       | 0.43          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB2  | 10       | 0.43          |
| (2,2005) | 1:67:A:LEU:H    | 1:66:A:ALA:HB3  | 10       | 0.43          |
| (2,1353) | 1:92:A:TYR:HB3  | 1:64:A:PHE:HB3  | 4        | 0.43          |
| (2,1096) | 1:38:A:VAL:HG21 | 1:37:A:ASP:HA   | 6        | 0.43          |
| (2,1096) | 1:38:A:VAL:HG22 | 1:37:A:ASP:HA   | 6        | 0.43          |
| (2,1096) | 1:38:A:VAL:HG23 | 1:37:A:ASP:HA   | 6        | 0.43          |
| (2,948)  | 1:111:A:LEU:HB2 | 1:112:A:HIS:HA  | 10       | 0.43          |
| (2,604)  | 1:38:A:VAL:HG21 | 1:47:A:ALA:HA   | 7        | 0.43          |
| (2,604)  | 1:38:A:VAL:HG22 | 1:47:A:ALA:HA   | 7        | 0.43          |
| (2,604)  | 1:38:A:VAL:HG23 | 1:47:A:ALA:HA   | 7        | 0.43          |
| (2,601)  | 1:38:A:VAL:HG21 | 1:48:A:LYS:H    | 1        | 0.43          |
| (2,601)  | 1:38:A:VAL:HG22 | 1:48:A:LYS:H    | 1        | 0.43          |
| (2,601)  | 1:38:A:VAL:HG23 | 1:48:A:LYS:H    | 1        | 0.43          |
| (2,2842) | 1:61:A:GLU:H    | 1:59:A:GLU:HB2  | 7        | 0.42          |
| (2,2831) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 2        | 0.42          |
| (2,1832) | 1:16:A:GLU:H    | 1:12:A:GLN:HB2  | 4        | 0.42          |
| (2,1765) | 1:109:A:GLN:H   | 1:110:A:ASP:HB3 | 9        | 0.42          |
| (2,1105) | 1:39:A:VAL:HG21 | 1:37:A:ASP:HB2  | 6        | 0.42          |
| (2,1105) | 1:39:A:VAL:HG22 | 1:37:A:ASP:HB2  | 6        | 0.42          |
| (2,1105) | 1:39:A:VAL:HG23 | 1:37:A:ASP:HB2  | 6        | 0.42          |
| (2,1102) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HA   | 6        | 0.42          |
| (2,1102) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HA   | 6        | 0.42          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1102) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HA   | 6        | 0.42          |
| (2,1098) | 1:38:A:VAL:HG21 | 1:17:A:LEU:H    | 9        | 0.42          |
| (2,1098) | 1:38:A:VAL:HG22 | 1:17:A:LEU:H    | 9        | 0.42          |
| (2,1098) | 1:38:A:VAL:HG23 | 1:17:A:LEU:H    | 9        | 0.42          |
| (2,638)  | 1:45:A:SER:HB3  | 1:46:A:GLN:HG2  | 8        | 0.42          |
| (2,146)  | 1:64:A:PHE:HA   | 1:67:A:LEU:HB2  | 4        | 0.42          |
| (2,2928) | 1:79:A:GLY:H    | 1:75:A:LYS:HB2  | 6        | 0.41          |
| (2,2928) | 1:79:A:GLY:H    | 1:75:A:LYS:HB2  | 8        | 0.41          |
| (2,2928) | 1:79:A:GLY:H    | 1:75:A:LYS:HB2  | 10       | 0.41          |
| (2,2877) | 1:69:A:LYS:H    | 1:65:A:LYS:HB2  | 5        | 0.41          |
| (2,2831) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 5        | 0.41          |
| (2,2831) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 9        | 0.41          |
| (2,2752) | 1:46:A:GLN:HE22 | 1:46:A:GLN:HA   | 7        | 0.41          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG21 | 2        | 0.41          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG22 | 2        | 0.41          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG23 | 2        | 0.41          |
| (2,2657) | 1:23:A:ASN:H    | 1:23:A:ASN:HD22 | 10       | 0.41          |
| (2,2358) | 1:41:A:THR:H    | 1:46:A:GLN:HA   | 10       | 0.41          |
| (2,1317) | 1:91:A:MET:HB2  | 1:48:A:LYS:HB3  | 10       | 0.41          |
| (2,1143) | 1:50:A:PHE:HB3  | 1:37:A:ASP:HB3  | 1        | 0.41          |
| (2,1102) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HA   | 3        | 0.41          |
| (2,1102) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HA   | 3        | 0.41          |
| (2,1102) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HA   | 3        | 0.41          |
| (2,1102) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HA   | 4        | 0.41          |
| (2,1102) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HA   | 4        | 0.41          |
| (2,1102) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HA   | 4        | 0.41          |
| (2,601)  | 1:38:A:VAL:HG21 | 1:48:A:LYS:H    | 9        | 0.41          |
| (2,601)  | 1:38:A:VAL:HG22 | 1:48:A:LYS:H    | 9        | 0.41          |
| (2,601)  | 1:38:A:VAL:HG23 | 1:48:A:LYS:H    | 9        | 0.41          |
| (2,2928) | 1:79:A:GLY:H    | 1:75:A:LYS:HB2  | 9        | 0.4           |
| (2,2881) | 1:70:A:ALA:H    | 1:71:A:LYS:HB3  | 5        | 0.4           |
| (2,2831) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 6        | 0.4           |
| (2,2831) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 10       | 0.4           |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD21 | 1        | 0.4           |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD22 | 1        | 0.4           |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD23 | 1        | 0.4           |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD21 | 4        | 0.4           |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD22 | 4        | 0.4           |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD23 | 4        | 0.4           |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD21 | 9        | 0.4           |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD22 | 9        | 0.4           |
| (2,1965) | 1:55:A:GLY:H    | 1:54:A:LEU:HD23 | 9        | 0.4           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1765) | 1:109:A:GLN:H   | 1:110:A:ASP:HB3 | 1        | 0.4           |
| (2,1765) | 1:109:A:GLN:H   | 1:110:A:ASP:HB3 | 4        | 0.4           |
| (2,1765) | 1:109:A:GLN:H   | 1:110:A:ASP:HB3 | 6        | 0.4           |
| (2,1576) | 1:58:A:LYS:H    | 1:61:A:GLU:HB2  | 6        | 0.4           |
| (2,1105) | 1:39:A:VAL:HG21 | 1:37:A:ASP:HB2  | 2        | 0.4           |
| (2,1105) | 1:39:A:VAL:HG22 | 1:37:A:ASP:HB2  | 2        | 0.4           |
| (2,1105) | 1:39:A:VAL:HG23 | 1:37:A:ASP:HB2  | 2        | 0.4           |
| (2,1105) | 1:39:A:VAL:HG21 | 1:37:A:ASP:HB2  | 7        | 0.4           |
| (2,1105) | 1:39:A:VAL:HG22 | 1:37:A:ASP:HB2  | 7        | 0.4           |
| (2,1105) | 1:39:A:VAL:HG23 | 1:37:A:ASP:HB2  | 7        | 0.4           |
| (2,1096) | 1:38:A:VAL:HG21 | 1:37:A:ASP:HA   | 5        | 0.4           |
| (2,1096) | 1:38:A:VAL:HG22 | 1:37:A:ASP:HA   | 5        | 0.4           |
| (2,1096) | 1:38:A:VAL:HG23 | 1:37:A:ASP:HA   | 5        | 0.4           |
| (2,932)  | 1:109:A:GLN:HB2 | 1:107:A:MET:HA  | 4        | 0.4           |
| (2,604)  | 1:38:A:VAL:HG21 | 1:47:A:ALA:HA   | 1        | 0.4           |
| (2,604)  | 1:38:A:VAL:HG22 | 1:47:A:ALA:HA   | 1        | 0.4           |
| (2,604)  | 1:38:A:VAL:HG23 | 1:47:A:ALA:HA   | 1        | 0.4           |
| (2,301)  | 1:91:A:MET:HB2  | 1:48:A:LYS:HA   | 2        | 0.4           |
| (2,215)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB3  | 2        | 0.4           |
| (2,215)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB3  | 2        | 0.4           |
| (2,215)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB3  | 2        | 0.4           |
| (2,2881) | 1:70:A:ALA:H    | 1:71:A:LYS:HB3  | 3        | 0.39          |
| (2,2877) | 1:69:A:LYS:H    | 1:65:A:LYS:HB2  | 2        | 0.39          |
| (2,2831) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 4        | 0.39          |
| (2,2358) | 1:41:A:THR:H    | 1:46:A:GLN:HA   | 8        | 0.39          |
| (2,2090) | 1:99:A:GLU:H    | 1:101:A:GLY:HA2 | 3        | 0.39          |
| (2,1765) | 1:109:A:GLN:H   | 1:110:A:ASP:HB3 | 2        | 0.39          |
| (2,1143) | 1:50:A:PHE:HB3  | 1:37:A:ASP:HB3  | 7        | 0.39          |
| (2,1102) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HA   | 1        | 0.39          |
| (2,1102) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HA   | 1        | 0.39          |
| (2,1102) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HA   | 1        | 0.39          |
| (2,941)  | 1:111:A:LEU:HA  | 1:110:A:ASP:H   | 7        | 0.39          |
| (2,938)  | 1:111:A:LEU:HA  | 1:113:A:LYS:HB3 | 2        | 0.39          |
| (2,526)  | 1:22:A:ASN:HA   | 1:22:A:ASN:HD22 | 2        | 0.39          |
| (2,301)  | 1:91:A:MET:HB2  | 1:48:A:LYS:HA   | 1        | 0.39          |
| (2,2869) | 1:68:A:ASP:H    | 1:92:A:TYR:HB3  | 7        | 0.38          |
| (2,2831) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 3        | 0.38          |
| (2,2831) | 1:59:A:GLU:H    | 1:56:A:ASN:HA   | 8        | 0.38          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG21 | 3        | 0.38          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG22 | 3        | 0.38          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG23 | 3        | 0.38          |
| (2,2038) | 1:76:A:SER:H    | 1:72:A:GLY:HA3  | 7        | 0.38          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1886) | 1:36:A:THR:H    | 1:37:A:ASP:HA   | 2        | 0.38          |
| (2,1886) | 1:36:A:THR:H    | 1:37:A:ASP:HA   | 10       | 0.38          |
| (2,1576) | 1:58:A:LYS:H    | 1:61:A:GLU:HB2  | 4        | 0.38          |
| (2,1576) | 1:58:A:LYS:H    | 1:61:A:GLU:HB2  | 9        | 0.38          |
| (2,1353) | 1:92:A:TYR:HB3  | 1:64:A:PHE:HB3  | 7        | 0.38          |
| (2,1317) | 1:91:A:MET:HB2  | 1:48:A:LYS:HB3  | 1        | 0.38          |
| (2,1143) | 1:50:A:PHE:HB3  | 1:37:A:ASP:HB3  | 6        | 0.38          |
| (2,1143) | 1:50:A:PHE:HB3  | 1:37:A:ASP:HB3  | 8        | 0.38          |
| (2,1106) | 1:39:A:VAL:HG21 | 1:48:A:LYS:HB3  | 4        | 0.38          |
| (2,1106) | 1:39:A:VAL:HG22 | 1:48:A:LYS:HB3  | 4        | 0.38          |
| (2,1106) | 1:39:A:VAL:HG23 | 1:48:A:LYS:HB3  | 4        | 0.38          |
| (2,1105) | 1:39:A:VAL:HG21 | 1:37:A:ASP:HB2  | 5        | 0.38          |
| (2,1105) | 1:39:A:VAL:HG22 | 1:37:A:ASP:HB2  | 5        | 0.38          |
| (2,1105) | 1:39:A:VAL:HG23 | 1:37:A:ASP:HB2  | 5        | 0.38          |
| (2,1102) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HA   | 7        | 0.38          |
| (2,1102) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HA   | 7        | 0.38          |
| (2,1102) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HA   | 7        | 0.38          |
| (2,950)  | 1:111:A:LEU:HB2 | 1:110:A:ASP:HB2 | 6        | 0.38          |
| (2,215)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB3  | 1        | 0.38          |
| (2,215)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB3  | 1        | 0.38          |
| (2,215)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB3  | 1        | 0.38          |
| (2,215)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB3  | 7        | 0.38          |
| (2,215)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB3  | 7        | 0.38          |
| (2,215)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB3  | 7        | 0.38          |
| (2,210)  | 1:78:A:LEU:HA   | 1:16:A:GLU:HB2  | 9        | 0.38          |
| (2,2928) | 1:79:A:GLY:H    | 1:75:A:LYS:HB2  | 4        | 0.37          |
| (2,2877) | 1:69:A:LYS:H    | 1:65:A:LYS:HB2  | 3        | 0.37          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG21 | 1        | 0.37          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG22 | 1        | 0.37          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG23 | 1        | 0.37          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG21 | 6        | 0.37          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG22 | 6        | 0.37          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG23 | 6        | 0.37          |
| (2,1886) | 1:36:A:THR:H    | 1:37:A:ASP:HA   | 8        | 0.37          |
| (2,1576) | 1:58:A:LYS:H    | 1:61:A:GLU:HB2  | 5        | 0.37          |
| (2,1508) | 1:47:A:ALA:H    | 1:91:A:MET:HB2  | 8        | 0.37          |
| (2,1102) | 1:39:A:VAL:HG21 | 1:40:A:LEU:HA   | 2        | 0.37          |
| (2,1102) | 1:39:A:VAL:HG22 | 1:40:A:LEU:HA   | 2        | 0.37          |
| (2,1102) | 1:39:A:VAL:HG23 | 1:40:A:LEU:HA   | 2        | 0.37          |
| (2,1098) | 1:38:A:VAL:HG21 | 1:17:A:LEU:H    | 5        | 0.37          |
| (2,1098) | 1:38:A:VAL:HG22 | 1:17:A:LEU:H    | 5        | 0.37          |
| (2,1098) | 1:38:A:VAL:HG23 | 1:17:A:LEU:H    | 5        | 0.37          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1092) | 1:38:A:VAL:HG21 | 1:17:A:LEU:HB3  | 6        | 0.37          |
| (2,1092) | 1:38:A:VAL:HG22 | 1:17:A:LEU:HB3  | 6        | 0.37          |
| (2,1092) | 1:38:A:VAL:HG23 | 1:17:A:LEU:HB3  | 6        | 0.37          |
| (2,941)  | 1:111:A:LEU:HA  | 1:110:A:ASP:H   | 9        | 0.37          |
| (2,2928) | 1:79:A:GLY:H    | 1:75:A:LYS:HB2  | 7        | 0.36          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG21 | 9        | 0.36          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG22 | 9        | 0.36          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG23 | 9        | 0.36          |
| (2,2358) | 1:41:A:THR:H    | 1:46:A:GLN:HA   | 3        | 0.36          |
| (2,1616) | 1:66:A:ALA:H    | 1:65:A:LYS:HD2  | 8        | 0.36          |
| (2,1317) | 1:91:A:MET:HB2  | 1:48:A:LYS:HB3  | 9        | 0.36          |
| (2,1143) | 1:50:A:PHE:HB3  | 1:37:A:ASP:HB3  | 9        | 0.36          |
| (2,1092) | 1:38:A:VAL:HG21 | 1:17:A:LEU:HB3  | 1        | 0.36          |
| (2,1092) | 1:38:A:VAL:HG22 | 1:17:A:LEU:HB3  | 1        | 0.36          |
| (2,1092) | 1:38:A:VAL:HG23 | 1:17:A:LEU:HB3  | 1        | 0.36          |
| (2,938)  | 1:111:A:LEU:HA  | 1:113:A:LYS:HB3 | 3        | 0.36          |
| (2,507)  | 1:19:A:ASP:HA   | 1:22:A:ASN:HB3  | 1        | 0.36          |
| (2,507)  | 1:19:A:ASP:HA   | 1:22:A:ASN:HB3  | 3        | 0.36          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG21 | 9        | 0.36          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG22 | 9        | 0.36          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG23 | 9        | 0.36          |
| (2,2881) | 1:70:A:ALA:H    | 1:71:A:LYS:HB3  | 7        | 0.35          |
| (2,2752) | 1:46:A:GLN:HE22 | 1:46:A:GLN:HA   | 5        | 0.35          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG21 | 4        | 0.35          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG22 | 4        | 0.35          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG23 | 4        | 0.35          |
| (2,2358) | 1:41:A:THR:H    | 1:46:A:GLN:HA   | 2        | 0.35          |
| (2,1924) | 1:45:A:SER:H    | 1:46:A:GLN:HA   | 1        | 0.35          |
| (2,1924) | 1:45:A:SER:H    | 1:46:A:GLN:HA   | 2        | 0.35          |
| (2,1353) | 1:92:A:TYR:HB3  | 1:64:A:PHE:HB3  | 2        | 0.35          |
| (2,1291) | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 2        | 0.35          |
| (2,1291) | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 10       | 0.35          |
| (2,1143) | 1:50:A:PHE:HB3  | 1:37:A:ASP:HB3  | 4        | 0.35          |
| (2,934)  | 1:109:A:GLN:HB2 | 1:110:A:ASP:HB2 | 6        | 0.35          |
| (2,604)  | 1:38:A:VAL:HG21 | 1:47:A:ALA:HA   | 10       | 0.35          |
| (2,604)  | 1:38:A:VAL:HG22 | 1:47:A:ALA:HA   | 10       | 0.35          |
| (2,604)  | 1:38:A:VAL:HG23 | 1:47:A:ALA:HA   | 10       | 0.35          |
| (2,216)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB2  | 9        | 0.35          |
| (2,216)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB2  | 9        | 0.35          |
| (2,216)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB2  | 9        | 0.35          |
| (2,121)  | 1:45:A:SER:HA   | 1:88:A:PRO:HA   | 8        | 0.35          |
| (2,2928) | 1:79:A:GLY:H    | 1:75:A:LYS:HB2  | 1        | 0.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2928) | 1:79:A:GLY:H    | 1:75:A:LYS:HB2  | 2        | 0.34          |
| (2,2869) | 1:68:A:ASP:H    | 1:92:A:TYR:HB3  | 5        | 0.34          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG21 | 7        | 0.34          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG22 | 7        | 0.34          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG23 | 7        | 0.34          |
| (2,2441) | 1:60:A:VAL:H    | 1:59:A:GLU:HG2  | 2        | 0.34          |
| (2,2358) | 1:41:A:THR:H    | 1:46:A:GLN:HA   | 9        | 0.34          |
| (2,2118) | 1:112:A:HIS:H   | 1:78:A:LEU:HB3  | 5        | 0.34          |
| (2,1353) | 1:92:A:TYR:HB3  | 1:64:A:PHE:HB3  | 8        | 0.34          |
| (2,1291) | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 1        | 0.34          |
| (2,1291) | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 8        | 0.34          |
| (2,1098) | 1:38:A:VAL:HG21 | 1:17:A:LEU:H    | 1        | 0.34          |
| (2,1098) | 1:38:A:VAL:HG22 | 1:17:A:LEU:H    | 1        | 0.34          |
| (2,1098) | 1:38:A:VAL:HG23 | 1:17:A:LEU:H    | 1        | 0.34          |
| (2,1092) | 1:38:A:VAL:HG21 | 1:17:A:LEU:HB3  | 9        | 0.34          |
| (2,1092) | 1:38:A:VAL:HG22 | 1:17:A:LEU:HB3  | 9        | 0.34          |
| (2,1092) | 1:38:A:VAL:HG23 | 1:17:A:LEU:HB3  | 9        | 0.34          |
| (2,932)  | 1:109:A:GLN:HB2 | 1:107:A:MET:HA  | 5        | 0.34          |
| (2,932)  | 1:109:A:GLN:HB2 | 1:107:A:MET:HA  | 10       | 0.34          |
| (2,919)  | 1:108:A:ILE:HA  | 1:110:A:ASP:HB2 | 3        | 0.34          |
| (2,616)  | 1:39:A:VAL:HG21 | 1:40:A:LEU:H    | 8        | 0.34          |
| (2,616)  | 1:39:A:VAL:HG22 | 1:40:A:LEU:H    | 8        | 0.34          |
| (2,616)  | 1:39:A:VAL:HG23 | 1:40:A:LEU:H    | 8        | 0.34          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG21 | 8        | 0.34          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG22 | 8        | 0.34          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG23 | 8        | 0.34          |
| (1,128)  | 1:21:A:ILE:O    | 1:25:A:VAL:H    | 6        | 0.34          |
| (1,128)  | 1:21:A:ILE:O    | 1:25:A:VAL:H    | 9        | 0.34          |
| (2,2928) | 1:79:A:GLY:H    | 1:75:A:LYS:HB2  | 5        | 0.33          |
| (2,2820) | 1:58:A:LYS:H    | 1:60:A:VAL:HB   | 3        | 0.33          |
| (2,2358) | 1:41:A:THR:H    | 1:46:A:GLN:HA   | 1        | 0.33          |
| (2,2358) | 1:41:A:THR:H    | 1:46:A:GLN:HA   | 6        | 0.33          |
| (2,1924) | 1:45:A:SER:H    | 1:46:A:GLN:HA   | 4        | 0.33          |
| (2,1599) | 1:62:A:ASN:H    | 1:64:A:PHE:HB3  | 2        | 0.33          |
| (2,1576) | 1:58:A:LYS:H    | 1:61:A:GLU:HB2  | 3        | 0.33          |
| (2,1576) | 1:58:A:LYS:H    | 1:61:A:GLU:HB2  | 10       | 0.33          |
| (2,1508) | 1:47:A:ALA:H    | 1:91:A:MET:HB2  | 7        | 0.33          |
| (2,1317) | 1:91:A:MET:HB2  | 1:48:A:LYS:HB3  | 2        | 0.33          |
| (2,1291) | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 9        | 0.33          |
| (2,1096) | 1:38:A:VAL:HG21 | 1:37:A:ASP:HA   | 1        | 0.33          |
| (2,1096) | 1:38:A:VAL:HG22 | 1:37:A:ASP:HA   | 1        | 0.33          |
| (2,1096) | 1:38:A:VAL:HG23 | 1:37:A:ASP:HA   | 1        | 0.33          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,950)  | 1:111:A:LEU:HB2 | 1:110:A:ASP:HB2 | 9        | 0.33          |
| (2,941)  | 1:111:A:LEU:HA  | 1:110:A:ASP:H   | 10       | 0.33          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB1  | 5        | 0.33          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB2  | 5        | 0.33          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB3  | 5        | 0.33          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB1  | 5        | 0.33          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB2  | 5        | 0.33          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB3  | 5        | 0.33          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB1  | 5        | 0.33          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB2  | 5        | 0.33          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB3  | 5        | 0.33          |
| (2,2907) | 1:75:A:LYS:H    | 1:76:A:SER:HB3  | 4        | 0.32          |
| (2,2820) | 1:58:A:LYS:H    | 1:60:A:VAL:HB   | 4        | 0.32          |
| (2,2820) | 1:58:A:LYS:H    | 1:60:A:VAL:HB   | 5        | 0.32          |
| (2,1924) | 1:45:A:SER:H    | 1:46:A:GLN:HA   | 10       | 0.32          |
| (2,1886) | 1:36:A:THR:H    | 1:37:A:ASP:HA   | 6        | 0.32          |
| (2,1508) | 1:47:A:ALA:H    | 1:91:A:MET:HB2  | 3        | 0.32          |
| (2,1092) | 1:38:A:VAL:HG21 | 1:17:A:LEU:HB3  | 4        | 0.32          |
| (2,1092) | 1:38:A:VAL:HG22 | 1:17:A:LEU:HB3  | 4        | 0.32          |
| (2,1092) | 1:38:A:VAL:HG23 | 1:17:A:LEU:HB3  | 4        | 0.32          |
| (2,1092) | 1:38:A:VAL:HG21 | 1:17:A:LEU:HB3  | 7        | 0.32          |
| (2,1092) | 1:38:A:VAL:HG22 | 1:17:A:LEU:HB3  | 7        | 0.32          |
| (2,1092) | 1:38:A:VAL:HG23 | 1:17:A:LEU:HB3  | 7        | 0.32          |
| (2,938)  | 1:111:A:LEU:HA  | 1:113:A:LYS:HB3 | 9        | 0.32          |
| (2,932)  | 1:109:A:GLN:HB2 | 1:107:A:MET:HA  | 7        | 0.32          |
| (2,932)  | 1:109:A:GLN:HB2 | 1:107:A:MET:HA  | 8        | 0.32          |
| (2,604)  | 1:38:A:VAL:HG21 | 1:47:A:ALA:HA   | 6        | 0.32          |
| (2,604)  | 1:38:A:VAL:HG22 | 1:47:A:ALA:HA   | 6        | 0.32          |
| (2,604)  | 1:38:A:VAL:HG23 | 1:47:A:ALA:HA   | 6        | 0.32          |
| (2,604)  | 1:38:A:VAL:HG21 | 1:47:A:ALA:HA   | 9        | 0.32          |
| (2,604)  | 1:38:A:VAL:HG22 | 1:47:A:ALA:HA   | 9        | 0.32          |
| (2,604)  | 1:38:A:VAL:HG23 | 1:47:A:ALA:HA   | 9        | 0.32          |
| (2,601)  | 1:38:A:VAL:HG21 | 1:48:A:LYS:H    | 8        | 0.32          |
| (2,601)  | 1:38:A:VAL:HG22 | 1:48:A:LYS:H    | 8        | 0.32          |
| (2,601)  | 1:38:A:VAL:HG23 | 1:48:A:LYS:H    | 8        | 0.32          |
| (2,369)  | 1:19:A:ASP:HA   | 1:23:A:ASN:HB3  | 10       | 0.32          |
| (2,2820) | 1:58:A:LYS:H    | 1:60:A:VAL:HB   | 7        | 0.31          |
| (2,2820) | 1:58:A:LYS:H    | 1:60:A:VAL:HB   | 8        | 0.31          |
| (2,2820) | 1:58:A:LYS:H    | 1:60:A:VAL:HB   | 9        | 0.31          |
| (2,2657) | 1:23:A:ASN:H    | 1:23:A:ASN:HD22 | 2        | 0.31          |
| (2,2358) | 1:41:A:THR:H    | 1:46:A:GLN:HA   | 4        | 0.31          |
| (2,2038) | 1:76:A:SER:H    | 1:72:A:GLY:HA3  | 6        | 0.31          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1924) | 1:45:A:SER:H    | 1:46:A:GLN:HA    | 8        | 0.31          |
| (2,1616) | 1:66:A:ALA:H    | 1:65:A:LYS:HD2   | 7        | 0.31          |
| (2,1576) | 1:58:A:LYS:H    | 1:61:A:GLU:HB2   | 8        | 0.31          |
| (2,1317) | 1:91:A:MET:HB2  | 1:48:A:LYS:HB3   | 6        | 0.31          |
| (2,948)  | 1:111:A:LEU:HB2 | 1:112:A:HIS:HA   | 4        | 0.31          |
| (2,941)  | 1:111:A:LEU:HA  | 1:110:A:ASP:H    | 4        | 0.31          |
| (2,938)  | 1:111:A:LEU:HA  | 1:113:A:LYS:HB3  | 4        | 0.31          |
| (2,919)  | 1:108:A:ILE:HA  | 1:110:A:ASP:HB2  | 10       | 0.31          |
| (2,369)  | 1:19:A:ASP:HA   | 1:23:A:ASN:HB3   | 7        | 0.31          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG21  | 10       | 0.31          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG22  | 10       | 0.31          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG23  | 10       | 0.31          |
| (1,128)  | 1:21:A:ILE:O    | 1:25:A:VAL:H     | 5        | 0.31          |
| (2,2886) | 1:71:A:LYS:H    | 1:69:A:LYS:HB3   | 5        | 0.3           |
| (2,2820) | 1:58:A:LYS:H    | 1:60:A:VAL:HB    | 1        | 0.3           |
| (2,2752) | 1:46:A:GLN:HE22 | 1:46:A:GLN:HA    | 9        | 0.3           |
| (2,2497) | 1:70:A:ALA:H    | 1:69:A:LYS:HD2   | 7        | 0.3           |
| (2,2441) | 1:60:A:VAL:H    | 1:59:A:GLU:HG2   | 1        | 0.3           |
| (2,2428) | 1:58:A:LYS:H    | 1:56:A:ASN:HA    | 1        | 0.3           |
| (2,2119) | 1:113:A:LYS:H   | 1:78:A:LEU:HB3   | 7        | 0.3           |
| (2,1924) | 1:45:A:SER:H    | 1:46:A:GLN:HA    | 3        | 0.3           |
| (2,1924) | 1:45:A:SER:H    | 1:46:A:GLN:HA    | 5        | 0.3           |
| (2,1886) | 1:36:A:THR:H    | 1:37:A:ASP:HA    | 3        | 0.3           |
| (2,1353) | 1:92:A:TYR:HB3  | 1:64:A:PHE:HB3   | 9        | 0.3           |
| (2,1291) | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3   | 4        | 0.3           |
| (2,1265) | 1:71:A:LYS:HB2  | 1:75:A:LYS:HG2   | 3        | 0.3           |
| (2,950)  | 1:111:A:LEU:HB2 | 1:110:A:ASP:HB2  | 7        | 0.3           |
| (2,948)  | 1:111:A:LEU:HB2 | 1:112:A:HIS:HA   | 3        | 0.3           |
| (2,931)  | 1:109:A:GLN:HB2 | 1:109:A:GLN:HE22 | 8        | 0.3           |
| (2,616)  | 1:39:A:VAL:HG21 | 1:40:A:LEU:H     | 5        | 0.3           |
| (2,616)  | 1:39:A:VAL:HG22 | 1:40:A:LEU:H     | 5        | 0.3           |
| (2,616)  | 1:39:A:VAL:HG23 | 1:40:A:LEU:H     | 5        | 0.3           |
| (2,301)  | 1:91:A:MET:HB2  | 1:48:A:LYS:HA    | 8        | 0.3           |
| (2,301)  | 1:91:A:MET:HB2  | 1:48:A:LYS:HA    | 10       | 0.3           |
| (2,210)  | 1:78:A:LEU:HA   | 1:16:A:GLU:HB2   | 7        | 0.3           |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG21  | 5        | 0.3           |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG22  | 5        | 0.3           |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG23  | 5        | 0.3           |
| (1,128)  | 1:21:A:ILE:O    | 1:25:A:VAL:H     | 8        | 0.3           |
| (2,2881) | 1:70:A:ALA:H    | 1:71:A:LYS:HB3   | 1        | 0.29          |
| (2,2881) | 1:70:A:ALA:H    | 1:71:A:LYS:HB3   | 10       | 0.29          |
| (2,2358) | 1:41:A:THR:H    | 1:46:A:GLN:HA    | 7        | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2096) | 1:102:A:ASN:H   | 1:101:A:GLY:HA2 | 10       | 0.29          |
| (2,2038) | 1:76:A:SER:H    | 1:72:A:GLY:HA3  | 10       | 0.29          |
| (2,1924) | 1:45:A:SER:H    | 1:46:A:GLN:HA   | 6        | 0.29          |
| (2,1886) | 1:36:A:THR:H    | 1:37:A:ASP:HA   | 5        | 0.29          |
| (2,1886) | 1:36:A:THR:H    | 1:37:A:ASP:HA   | 7        | 0.29          |
| (2,1508) | 1:47:A:ALA:H    | 1:91:A:MET:HB2  | 5        | 0.29          |
| (2,1143) | 1:50:A:PHE:HB3  | 1:37:A:ASP:HB3  | 5        | 0.29          |
| (2,1096) | 1:38:A:VAL:HG21 | 1:37:A:ASP:HA   | 9        | 0.29          |
| (2,1096) | 1:38:A:VAL:HG22 | 1:37:A:ASP:HA   | 9        | 0.29          |
| (2,1096) | 1:38:A:VAL:HG23 | 1:37:A:ASP:HA   | 9        | 0.29          |
| (2,1031) | 1:24:A:LYS:HB2  | 1:25:A:VAL:HG11 | 4        | 0.29          |
| (2,1031) | 1:24:A:LYS:HB2  | 1:25:A:VAL:HG12 | 4        | 0.29          |
| (2,1031) | 1:24:A:LYS:HB2  | 1:25:A:VAL:HG13 | 4        | 0.29          |
| (2,852)  | 1:75:A:LYS:HG2  | 1:72:A:GLY:HA3  | 5        | 0.29          |
| (2,851)  | 1:75:A:LYS:HG2  | 1:72:A:GLY:HA3  | 5        | 0.29          |
| (2,585)  | 1:37:A:ASP:HA   | 1:38:A:VAL:H    | 9        | 0.29          |
| (2,369)  | 1:19:A:ASP:HA   | 1:23:A:ASN:HB3  | 2        | 0.29          |
| (2,210)  | 1:78:A:LEU:HA   | 1:16:A:GLU:HB2  | 5        | 0.29          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB1  | 6        | 0.29          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB2  | 6        | 0.29          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB3  | 6        | 0.29          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB1  | 6        | 0.29          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB2  | 6        | 0.29          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB3  | 6        | 0.29          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB1  | 6        | 0.29          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB2  | 6        | 0.29          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB3  | 6        | 0.29          |
| (1,128)  | 1:21:A:ILE:O    | 1:25:A:VAL:H    | 2        | 0.29          |
| (1,128)  | 1:21:A:ILE:O    | 1:25:A:VAL:H    | 7        | 0.29          |
| (2,2991) | 1:98:A:ILE:H    | 1:99:A:GLU:HA   | 8        | 0.28          |
| (2,2752) | 1:46:A:GLN:HE22 | 1:46:A:GLN:HA   | 3        | 0.28          |
| (2,2214) | 1:76:A:SER:H    | 1:78:A:LEU:HB2  | 6        | 0.28          |
| (2,2096) | 1:102:A:ASN:H   | 1:101:A:GLY:HA2 | 3        | 0.28          |
| (2,1924) | 1:45:A:SER:H    | 1:46:A:GLN:HA   | 7        | 0.28          |
| (2,1924) | 1:45:A:SER:H    | 1:46:A:GLN:HA   | 9        | 0.28          |
| (2,1886) | 1:36:A:THR:H    | 1:37:A:ASP:HA   | 1        | 0.28          |
| (2,1849) | 1:21:A:ILE:H    | 1:25:A:VAL:HB   | 8        | 0.28          |
| (2,1616) | 1:66:A:ALA:H    | 1:65:A:LYS:HD2  | 2        | 0.28          |
| (2,1576) | 1:58:A:LYS:H    | 1:61:A:GLU:HB2  | 1        | 0.28          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD21 | 3        | 0.28          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD22 | 3        | 0.28          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD23 | 3        | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1291) | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 3        | 0.28          |
| (2,1291) | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 5        | 0.28          |
| (2,1291) | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 7        | 0.28          |
| (2,1143) | 1:50:A:PHE:HB3  | 1:37:A:ASP:HB3  | 2        | 0.28          |
| (2,1143) | 1:50:A:PHE:HB3  | 1:37:A:ASP:HB3  | 10       | 0.28          |
| (2,1092) | 1:38:A:VAL:HG21 | 1:17:A:LEU:HB3  | 3        | 0.28          |
| (2,1092) | 1:38:A:VAL:HG22 | 1:17:A:LEU:HB3  | 3        | 0.28          |
| (2,1092) | 1:38:A:VAL:HG23 | 1:17:A:LEU:HB3  | 3        | 0.28          |
| (2,919)  | 1:108:A:ILE:HA  | 1:110:A:ASP:HB2 | 1        | 0.28          |
| (2,616)  | 1:39:A:VAL:HG21 | 1:40:A:LEU:H    | 10       | 0.28          |
| (2,616)  | 1:39:A:VAL:HG22 | 1:40:A:LEU:H    | 10       | 0.28          |
| (2,616)  | 1:39:A:VAL:HG23 | 1:40:A:LEU:H    | 10       | 0.28          |
| (2,369)  | 1:19:A:ASP:HA   | 1:23:A:ASN:HB3  | 4        | 0.28          |
| (2,301)  | 1:91:A:MET:HB2  | 1:48:A:LYS:HA   | 4        | 0.28          |
| (2,239)  | 1:50:A:PHE:HB3  | 1:95:A:ASP:HA   | 2        | 0.28          |
| (2,215)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB3  | 3        | 0.28          |
| (2,215)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB3  | 3        | 0.28          |
| (2,215)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB3  | 3        | 0.28          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB1  | 8        | 0.28          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB2  | 8        | 0.28          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB3  | 8        | 0.28          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB1  | 8        | 0.28          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB2  | 8        | 0.28          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB3  | 8        | 0.28          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB1  | 8        | 0.28          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB2  | 8        | 0.28          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB3  | 8        | 0.28          |
| (2,126)  | 1:93:A:GLU:H    | 1:50:A:PHE:HA   | 8        | 0.28          |
| (2,121)  | 1:45:A:SER:HA   | 1:88:A:PRO:HA   | 7        | 0.28          |
| (2,79)   | 1:70:A:ALA:C    | 1:74:A:ILE:H    | 7        | 0.28          |
| (1,128)  | 1:21:A:ILE:O    | 1:25:A:VAL:H    | 1        | 0.28          |
| (2,3006) | 1:101:A:GLY:H   | 1:100:A:TYR:HA  | 8        | 0.27          |
| (2,2881) | 1:70:A:ALA:H    | 1:71:A:LYS:HB3  | 4        | 0.27          |
| (2,2820) | 1:58:A:LYS:H    | 1:60:A:VAL:HB   | 10       | 0.27          |
| (2,2752) | 1:46:A:GLN:HE22 | 1:46:A:GLN:HA   | 4        | 0.27          |
| (2,2358) | 1:41:A:THR:H    | 1:46:A:GLN:HA   | 5        | 0.27          |
| (2,2118) | 1:112:A:HIS:H   | 1:78:A:LEU:HB3  | 8        | 0.27          |
| (2,1997) | 1:63:A:THR:H    | 1:62:A:ASN:HA   | 4        | 0.27          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG21 | 1        | 0.27          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG22 | 1        | 0.27          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG23 | 1        | 0.27          |
| (2,1886) | 1:36:A:THR:H    | 1:37:A:ASP:HA   | 4        | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1876) | 1:34:A:THR:H    | 1:52:A:THR:HB   | 7        | 0.27          |
| (2,1832) | 1:16:A:GLU:H    | 1:12:A:GLN:HB2  | 10       | 0.27          |
| (2,1814) | 1:14:A:LYS:H    | 1:12:A:GLN:HB2  | 3        | 0.27          |
| (2,1765) | 1:109:A:GLN:H   | 1:110:A:ASP:HB3 | 3        | 0.27          |
| (2,1576) | 1:58:A:LYS:H    | 1:61:A:GLU:HB2  | 7        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD21 | 1        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD22 | 1        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD23 | 1        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD21 | 5        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD22 | 5        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD23 | 5        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD21 | 7        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD22 | 7        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD23 | 7        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD21 | 8        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD22 | 8        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD23 | 8        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD21 | 9        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD22 | 9        | 0.27          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD23 | 9        | 0.27          |
| (2,1271) | 1:71:A:LYS:HB3  | 1:75:A:LYS:HG2  | 5        | 0.27          |
| (2,960)  | 1:118:A:GLU:HA  | 1:117:A:VAL:HB  | 3        | 0.27          |
| (2,941)  | 1:111:A:LEU:HA  | 1:110:A:ASP:H   | 6        | 0.27          |
| (2,934)  | 1:109:A:GLN:HB2 | 1:110:A:ASP:HB2 | 9        | 0.27          |
| (2,919)  | 1:108:A:ILE:HA  | 1:110:A:ASP:HB2 | 8        | 0.27          |
| (2,585)  | 1:37:A:ASP:HA   | 1:38:A:VAL:H    | 1        | 0.27          |
| (2,271)  | 1:50:A:PHE:HA   | 1:51:A:LEU:H    | 3        | 0.27          |
| (2,271)  | 1:50:A:PHE:HA   | 1:51:A:LEU:H    | 10       | 0.27          |
| (2,234)  | 1:49:A:VAL:HG21 | 1:35:A:ILE:HA   | 7        | 0.27          |
| (2,234)  | 1:49:A:VAL:HG22 | 1:35:A:ILE:HA   | 7        | 0.27          |
| (2,234)  | 1:49:A:VAL:HG23 | 1:35:A:ILE:HA   | 7        | 0.27          |
| (2,208)  | 1:79:A:GLY:HA2  | 1:76:A:SER:HA   | 6        | 0.27          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG21 | 6        | 0.27          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG22 | 6        | 0.27          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG23 | 6        | 0.27          |
| (2,80)   | 1:70:A:ALA:C    | 1:74:A:ILE:N    | 7        | 0.27          |
| (2,2118) | 1:112:A:HIS:H   | 1:78:A:LEU:HB3  | 7        | 0.26          |
| (2,1508) | 1:47:A:ALA:H    | 1:91:A:MET:HB2  | 1        | 0.26          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD21 | 4        | 0.26          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD22 | 4        | 0.26          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD23 | 4        | 0.26          |
| (2,1389) | 1:15:A:LYS:H    | 1:16:A:GLU:HB2  | 8        | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1353) | 1:92:A:TYR:HB3  | 1:64:A:PHE:HB3  | 1        | 0.26          |
| (2,1353) | 1:92:A:TYR:HB3  | 1:64:A:PHE:HB3  | 3        | 0.26          |
| (2,1344) | 1:98:A:ILE:HG12 | 1:95:A:ASP:HB2  | 2        | 0.26          |
| (2,1291) | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 6        | 0.26          |
| (2,948)  | 1:111:A:LEU:HB2 | 1:112:A:HIS:HA  | 7        | 0.26          |
| (2,919)  | 1:108:A:ILE:HA  | 1:110:A:ASP:HB2 | 2        | 0.26          |
| (2,883)  | 1:81:A:ARG:HB3  | 1:80:A:SER:H    | 10       | 0.26          |
| (2,604)  | 1:38:A:VAL:HG21 | 1:47:A:ALA:HA   | 5        | 0.26          |
| (2,604)  | 1:38:A:VAL:HG22 | 1:47:A:ALA:HA   | 5        | 0.26          |
| (2,604)  | 1:38:A:VAL:HG23 | 1:47:A:ALA:HA   | 5        | 0.26          |
| (2,585)  | 1:37:A:ASP:HA   | 1:38:A:VAL:H    | 8        | 0.26          |
| (2,301)  | 1:91:A:MET:HB2  | 1:48:A:LYS:HA   | 5        | 0.26          |
| (2,192)  | 1:25:A:VAL:HG21 | 1:74:A:ILE:HA   | 9        | 0.26          |
| (2,192)  | 1:25:A:VAL:HG22 | 1:74:A:ILE:HA   | 9        | 0.26          |
| (2,192)  | 1:25:A:VAL:HG23 | 1:74:A:ILE:HA   | 9        | 0.26          |
| (1,128)  | 1:21:A:ILE:O    | 1:25:A:VAL:H    | 3        | 0.26          |
| (2,2820) | 1:58:A:LYS:H    | 1:60:A:VAL:HB   | 6        | 0.25          |
| (2,2758) | 1:47:A:ALA:H    | 1:89:A:GLU:HB3  | 3        | 0.25          |
| (2,2650) | 1:22:A:ASN:H    | 1:18:A:MET:HA   | 9        | 0.25          |
| (2,2214) | 1:76:A:SER:H    | 1:78:A:LEU:HB2  | 7        | 0.25          |
| (2,2096) | 1:102:A:ASN:H   | 1:101:A:GLY:HA2 | 6        | 0.25          |
| (2,2088) | 1:99:A:GLU:H    | 1:98:A:ILE:HG13 | 4        | 0.25          |
| (2,2088) | 1:99:A:GLU:H    | 1:98:A:ILE:HG13 | 10       | 0.25          |
| (2,1814) | 1:14:A:LYS:H    | 1:12:A:GLN:HB2  | 5        | 0.25          |
| (2,1784) | 1:12:A:GLN:HE22 | 1:12:A:GLN:HA   | 7        | 0.25          |
| (2,1765) | 1:109:A:GLN:H   | 1:110:A:ASP:HB3 | 10       | 0.25          |
| (2,1688) | 1:77:A:GLU:H    | 1:73:A:PHE:HA   | 7        | 0.25          |
| (2,1508) | 1:47:A:ALA:H    | 1:91:A:MET:HB2  | 10       | 0.25          |
| (2,1317) | 1:91:A:MET:HB2  | 1:48:A:LYS:HB3  | 5        | 0.25          |
| (2,1265) | 1:71:A:LYS:HB2  | 1:75:A:LYS:HG2  | 7        | 0.25          |
| (2,1118) | 1:46:A:GLN:HB2  | 1:41:A:THR:HG1  | 8        | 0.25          |
| (2,948)  | 1:111:A:LEU:HB2 | 1:112:A:HIS:HA  | 5        | 0.25          |
| (2,941)  | 1:111:A:LEU:HA  | 1:110:A:ASP:H   | 8        | 0.25          |
| (2,883)  | 1:81:A:ARG:HB3  | 1:80:A:SER:H    | 3        | 0.25          |
| (2,585)  | 1:37:A:ASP:HA   | 1:38:A:VAL:H    | 2        | 0.25          |
| (2,585)  | 1:37:A:ASP:HA   | 1:38:A:VAL:H    | 3        | 0.25          |
| (2,585)  | 1:37:A:ASP:HA   | 1:38:A:VAL:H    | 6        | 0.25          |
| (2,526)  | 1:22:A:ASN:HA   | 1:22:A:ASN:HD22 | 1        | 0.25          |
| (2,369)  | 1:19:A:ASP:HA   | 1:23:A:ASN:HB3  | 8        | 0.25          |
| (2,271)  | 1:50:A:PHE:HA   | 1:51:A:LEU:H    | 1        | 0.25          |
| (2,271)  | 1:50:A:PHE:HA   | 1:51:A:LEU:H    | 2        | 0.25          |
| (2,271)  | 1:50:A:PHE:HA   | 1:51:A:LEU:H    | 7        | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,216)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB2  | 8        | 0.25          |
| (2,216)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB2  | 8        | 0.25          |
| (2,216)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB2  | 8        | 0.25          |
| (2,210)  | 1:78:A:LEU:HA   | 1:16:A:GLU:HB2  | 6        | 0.25          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG21 | 2        | 0.25          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG22 | 2        | 0.25          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG23 | 2        | 0.25          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB1  | 9        | 0.25          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB2  | 9        | 0.25          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB3  | 9        | 0.25          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB1  | 9        | 0.25          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB2  | 9        | 0.25          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB3  | 9        | 0.25          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB1  | 9        | 0.25          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB2  | 9        | 0.25          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB3  | 9        | 0.25          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB1  | 10       | 0.25          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB2  | 10       | 0.25          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB3  | 10       | 0.25          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB1  | 10       | 0.25          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB2  | 10       | 0.25          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB3  | 10       | 0.25          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB1  | 10       | 0.25          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB2  | 10       | 0.25          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB3  | 10       | 0.25          |
| (2,136)  | 1:31:A:GLY:HA2  | 1:54:A:LEU:HB3  | 5        | 0.25          |
| (2,125)  | 1:49:A:VAL:H    | 1:92:A:TYR:HA   | 3        | 0.25          |
| (2,121)  | 1:45:A:SER:HA   | 1:88:A:PRO:HA   | 9        | 0.25          |
| (2,19)   | 1:12:A:GLN:C    | 1:16:A:GLU:H    | 7        | 0.25          |
| (1,137)  | 1:48:A:LYS:O    | 1:39:A:VAL:H    | 3        | 0.25          |
| (2,3006) | 1:101:A:GLY:H   | 1:100:A:TYR:HA  | 3        | 0.24          |
| (2,3006) | 1:101:A:GLY:H   | 1:100:A:TYR:HA  | 6        | 0.24          |
| (2,3006) | 1:101:A:GLY:H   | 1:100:A:TYR:HA  | 7        | 0.24          |
| (2,2913) | 1:77:A:GLU:H    | 1:78:A:LEU:HB2  | 1        | 0.24          |
| (2,2650) | 1:22:A:ASN:H    | 1:18:A:MET:HA   | 8        | 0.24          |
| (2,2118) | 1:112:A:HIS:H   | 1:78:A:LEU:HB3  | 4        | 0.24          |
| (2,2040) | 1:76:A:SER:H    | 1:77:A:GLU:HB3  | 10       | 0.24          |
| (2,2038) | 1:76:A:SER:H    | 1:72:A:GLY:HA3  | 9        | 0.24          |
| (2,1822) | 1:15:A:LYS:H    | 1:12:A:GLN:HB2  | 4        | 0.24          |
| (2,1822) | 1:15:A:LYS:H    | 1:12:A:GLN:HB2  | 10       | 0.24          |
| (2,1599) | 1:62:A:ASN:H    | 1:64:A:PHE:HB3  | 8        | 0.24          |
| (2,1599) | 1:62:A:ASN:H    | 1:64:A:PHE:HB3  | 9        | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1508) | 1:47:A:ALA:H    | 1:91:A:MET:HB2  | 6        | 0.24          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD21 | 10       | 0.24          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD22 | 10       | 0.24          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD23 | 10       | 0.24          |
| (2,1344) | 1:98:A:ILE:HG12 | 1:95:A:ASP:HB2  | 1        | 0.24          |
| (2,1344) | 1:98:A:ILE:HG12 | 1:95:A:ASP:HB2  | 4        | 0.24          |
| (2,1265) | 1:71:A:LYS:HB2  | 1:75:A:LYS:HG2  | 9        | 0.24          |
| (2,1216) | 1:62:A:ASN:HA   | 1:65:A:LYS:HD2  | 7        | 0.24          |
| (2,585)  | 1:37:A:ASP:HA   | 1:38:A:VAL:H    | 4        | 0.24          |
| (2,585)  | 1:37:A:ASP:HA   | 1:38:A:VAL:H    | 7        | 0.24          |
| (2,585)  | 1:37:A:ASP:HA   | 1:38:A:VAL:H    | 10       | 0.24          |
| (2,271)  | 1:50:A:PHE:HA   | 1:51:A:LEU:H    | 5        | 0.24          |
| (2,271)  | 1:50:A:PHE:HA   | 1:51:A:LEU:H    | 6        | 0.24          |
| (2,271)  | 1:50:A:PHE:HA   | 1:51:A:LEU:H    | 8        | 0.24          |
| (2,271)  | 1:50:A:PHE:HA   | 1:51:A:LEU:H    | 9        | 0.24          |
| (2,234)  | 1:49:A:VAL:HG21 | 1:35:A:ILE:HA   | 9        | 0.24          |
| (2,234)  | 1:49:A:VAL:HG22 | 1:35:A:ILE:HA   | 9        | 0.24          |
| (2,234)  | 1:49:A:VAL:HG23 | 1:35:A:ILE:HA   | 9        | 0.24          |
| (2,192)  | 1:25:A:VAL:HG21 | 1:74:A:ILE:HA   | 8        | 0.24          |
| (2,192)  | 1:25:A:VAL:HG22 | 1:74:A:ILE:HA   | 8        | 0.24          |
| (2,192)  | 1:25:A:VAL:HG23 | 1:74:A:ILE:HA   | 8        | 0.24          |
| (2,25)   | 1:15:A:LYS:C    | 1:19:A:ASP:H    | 1        | 0.24          |
| (2,25)   | 1:15:A:LYS:C    | 1:19:A:ASP:H    | 3        | 0.24          |
| (2,25)   | 1:15:A:LYS:C    | 1:19:A:ASP:H    | 7        | 0.24          |
| (1,127)  | 1:20:A:ILE:O    | 1:24:A:LYS:H    | 5        | 0.24          |
| (2,3006) | 1:101:A:GLY:H   | 1:100:A:TYR:HA  | 10       | 0.23          |
| (2,2959) | 1:91:A:MET:H    | 1:47:A:ALA:HA   | 5        | 0.23          |
| (2,2820) | 1:58:A:LYS:H    | 1:60:A:VAL:HB   | 2        | 0.23          |
| (2,2681) | 1:34:A:THR:H    | 1:51:A:LEU:HB2  | 1        | 0.23          |
| (2,2588) | 1:22:A:ASN:H    | 1:22:A:ASN:HD22 | 3        | 0.23          |
| (2,2428) | 1:58:A:LYS:H    | 1:56:A:ASN:HA   | 5        | 0.23          |
| (2,2214) | 1:76:A:SER:H    | 1:78:A:LEU:HB2  | 5        | 0.23          |
| (2,2119) | 1:113:A:LYS:H   | 1:78:A:LEU:HB3  | 8        | 0.23          |
| (2,2096) | 1:102:A:ASN:H   | 1:101:A:GLY:HA2 | 9        | 0.23          |
| (2,1997) | 1:63:A:THR:H    | 1:62:A:ASN:HA   | 7        | 0.23          |
| (2,1508) | 1:47:A:ALA:H    | 1:91:A:MET:HB2  | 2        | 0.23          |
| (2,1508) | 1:47:A:ALA:H    | 1:91:A:MET:HB2  | 9        | 0.23          |
| (2,1389) | 1:15:A:LYS:H    | 1:16:A:GLU:HB2  | 7        | 0.23          |
| (2,1344) | 1:98:A:ILE:HG12 | 1:95:A:ASP:HB2  | 7        | 0.23          |
| (2,934)  | 1:109:A:GLN:HB2 | 1:110:A:ASP:HB2 | 4        | 0.23          |
| (2,932)  | 1:109:A:GLN:HB2 | 1:107:A:MET:HA  | 1        | 0.23          |
| (2,883)  | 1:81:A:ARG:HB3  | 1:80:A:SER:H    | 6        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,723)  | 1:57:A:ASP:HB2  | 1:56:A:ASN:HB2  | 8        | 0.23          |
| (2,582)  | 1:36:A:THR:HG21 | 1:51:A:LEU:H    | 8        | 0.23          |
| (2,582)  | 1:36:A:THR:HG22 | 1:51:A:LEU:H    | 8        | 0.23          |
| (2,582)  | 1:36:A:THR:HG23 | 1:51:A:LEU:H    | 8        | 0.23          |
| (2,528)  | 1:22:A:ASN:HA   | 1:33:A:ILE:HB   | 10       | 0.23          |
| (2,526)  | 1:22:A:ASN:HA   | 1:22:A:ASN:HD22 | 3        | 0.23          |
| (2,510)  | 1:19:A:ASP:HA   | 1:18:A:MET:HA   | 8        | 0.23          |
| (2,301)  | 1:91:A:MET:HB2  | 1:48:A:LYS:HA   | 7        | 0.23          |
| (2,239)  | 1:50:A:PHE:HB3  | 1:95:A:ASP:HA   | 10       | 0.23          |
| (2,234)  | 1:49:A:VAL:HG21 | 1:35:A:ILE:HA   | 10       | 0.23          |
| (2,234)  | 1:49:A:VAL:HG22 | 1:35:A:ILE:HA   | 10       | 0.23          |
| (2,234)  | 1:49:A:VAL:HG23 | 1:35:A:ILE:HA   | 10       | 0.23          |
| (2,210)  | 1:78:A:LEU:HA   | 1:16:A:GLU:HB2  | 10       | 0.23          |
| (2,208)  | 1:79:A:GLY:HA2  | 1:76:A:SER:HA   | 1        | 0.23          |
| (2,208)  | 1:79:A:GLY:HA2  | 1:76:A:SER:HA   | 4        | 0.23          |
| (2,125)  | 1:49:A:VAL:H    | 1:92:A:TYR:HA   | 1        | 0.23          |
| (2,125)  | 1:49:A:VAL:H    | 1:92:A:TYR:HA   | 6        | 0.23          |
| (2,125)  | 1:49:A:VAL:H    | 1:92:A:TYR:HA   | 10       | 0.23          |
| (2,26)   | 1:15:A:LYS:C    | 1:19:A:ASP:N    | 1        | 0.23          |
| (2,20)   | 1:12:A:GLN:C    | 1:16:A:GLU:N    | 7        | 0.23          |
| (2,19)   | 1:12:A:GLN:C    | 1:16:A:GLU:H    | 1        | 0.23          |
| (2,19)   | 1:12:A:GLN:C    | 1:16:A:GLU:H    | 5        | 0.23          |
| (1,149)  | 1:70:A:ALA:O    | 1:74:A:ILE:H    | 7        | 0.23          |
| (2,3006) | 1:101:A:GLY:H   | 1:100:A:TYR:HA  | 9        | 0.22          |
| (2,2912) | 1:76:A:SER:H    | 1:77:A:GLU:HB3  | 5        | 0.22          |
| (2,2681) | 1:34:A:THR:H    | 1:51:A:LEU:HB2  | 5        | 0.22          |
| (2,2268) | 1:17:A:LEU:H    | 1:15:A:LYS:HB2  | 2        | 0.22          |
| (2,2268) | 1:17:A:LEU:H    | 1:15:A:LYS:HB2  | 6        | 0.22          |
| (2,2214) | 1:76:A:SER:H    | 1:78:A:LEU:HB2  | 9        | 0.22          |
| (2,2090) | 1:99:A:GLU:H    | 1:101:A:GLY:HA2 | 8        | 0.22          |
| (2,1997) | 1:63:A:THR:H    | 1:62:A:ASN:HA   | 1        | 0.22          |
| (2,1997) | 1:63:A:THR:H    | 1:62:A:ASN:HA   | 2        | 0.22          |
| (2,1997) | 1:63:A:THR:H    | 1:62:A:ASN:HA   | 6        | 0.22          |
| (2,1997) | 1:63:A:THR:H    | 1:62:A:ASN:HA   | 8        | 0.22          |
| (2,1997) | 1:63:A:THR:H    | 1:62:A:ASN:HA   | 9        | 0.22          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG21 | 6        | 0.22          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG22 | 6        | 0.22          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG23 | 6        | 0.22          |
| (2,1876) | 1:34:A:THR:H    | 1:52:A:THR:HB   | 1        | 0.22          |
| (2,1616) | 1:66:A:ALA:H    | 1:65:A:LYS:HD2  | 1        | 0.22          |
| (2,1353) | 1:92:A:TYR:HB3  | 1:64:A:PHE:HB3  | 5        | 0.22          |
| (2,1353) | 1:92:A:TYR:HB3  | 1:64:A:PHE:HB3  | 6        | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1265) | 1:71:A:LYS:HB2  | 1:75:A:LYS:HG2  | 6        | 0.22          |
| (2,1247) | 1:68:A:ASP:HB2  | 1:71:A:LYS:HG3  | 2        | 0.22          |
| (2,919)  | 1:108:A:ILE:HA  | 1:110:A:ASP:HB2 | 5        | 0.22          |
| (2,883)  | 1:81:A:ARG:HB3  | 1:80:A:SER:H    | 9        | 0.22          |
| (2,601)  | 1:38:A:VAL:HG21 | 1:48:A:LYS:H    | 10       | 0.22          |
| (2,601)  | 1:38:A:VAL:HG22 | 1:48:A:LYS:H    | 10       | 0.22          |
| (2,601)  | 1:38:A:VAL:HG23 | 1:48:A:LYS:H    | 10       | 0.22          |
| (2,216)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB2  | 4        | 0.22          |
| (2,216)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB2  | 4        | 0.22          |
| (2,216)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB2  | 4        | 0.22          |
| (2,210)  | 1:78:A:LEU:HA   | 1:16:A:GLU:HB2  | 8        | 0.22          |
| (2,208)  | 1:79:A:GLY:HA2  | 1:76:A:SER:HA   | 2        | 0.22          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG21 | 4        | 0.22          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG22 | 4        | 0.22          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG23 | 4        | 0.22          |
| (2,136)  | 1:31:A:GLY:HA2  | 1:54:A:LEU:HB3  | 6        | 0.22          |
| (2,136)  | 1:31:A:GLY:HA2  | 1:54:A:LEU:HB3  | 7        | 0.22          |
| (2,26)   | 1:15:A:LYS:C    | 1:19:A:ASP:N    | 3        | 0.22          |
| (2,26)   | 1:15:A:LYS:C    | 1:19:A:ASP:N    | 7        | 0.22          |
| (2,3006) | 1:101:A:GLY:H   | 1:100:A:TYR:HA  | 5        | 0.21          |
| (2,2991) | 1:98:A:ILE:H    | 1:99:A:GLU:HA   | 2        | 0.21          |
| (2,2991) | 1:98:A:ILE:H    | 1:99:A:GLU:HA   | 5        | 0.21          |
| (2,2959) | 1:91:A:MET:H    | 1:47:A:ALA:HA   | 4        | 0.21          |
| (2,2899) | 1:74:A:ILE:H    | 1:71:A:LYS:HB3  | 4        | 0.21          |
| (2,2886) | 1:71:A:LYS:H    | 1:69:A:LYS:HB3  | 2        | 0.21          |
| (2,2856) | 1:63:A:THR:H    | 1:65:A:LYS:HG2  | 3        | 0.21          |
| (2,2657) | 1:23:A:ASN:H    | 1:23:A:ASN:HD22 | 1        | 0.21          |
| (2,2428) | 1:58:A:LYS:H    | 1:56:A:ASN:HA   | 7        | 0.21          |
| (2,1997) | 1:63:A:THR:H    | 1:62:A:ASN:HA   | 3        | 0.21          |
| (2,1997) | 1:63:A:THR:H    | 1:62:A:ASN:HA   | 5        | 0.21          |
| (2,1508) | 1:47:A:ALA:H    | 1:91:A:MET:HB2  | 4        | 0.21          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD21 | 2        | 0.21          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD22 | 2        | 0.21          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD23 | 2        | 0.21          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD21 | 6        | 0.21          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD22 | 6        | 0.21          |
| (2,1444) | 1:31:A:GLY:H    | 1:54:A:LEU:HD23 | 6        | 0.21          |
| (2,1389) | 1:15:A:LYS:H    | 1:16:A:GLU:HB2  | 9        | 0.21          |
| (2,1199) | 1:59:A:GLU:HB2  | 1:56:A:ASN:HD22 | 8        | 0.21          |
| (2,1101) | 1:39:A:VAL:HG21 | 1:50:A:PHE:HD1  | 4        | 0.21          |
| (2,1101) | 1:39:A:VAL:HG21 | 1:50:A:PHE:HD2  | 4        | 0.21          |
| (2,1101) | 1:39:A:VAL:HG22 | 1:50:A:PHE:HD1  | 4        | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1101) | 1:39:A:VAL:HG22 | 1:50:A:PHE:HD2  | 4        | 0.21          |
| (2,1101) | 1:39:A:VAL:HG23 | 1:50:A:PHE:HD1  | 4        | 0.21          |
| (2,1101) | 1:39:A:VAL:HG23 | 1:50:A:PHE:HD2  | 4        | 0.21          |
| (2,1093) | 1:38:A:VAL:HG21 | 1:10:A:GLY:HA3  | 8        | 0.21          |
| (2,1093) | 1:38:A:VAL:HG22 | 1:10:A:GLY:HA3  | 8        | 0.21          |
| (2,1093) | 1:38:A:VAL:HG23 | 1:10:A:GLY:HA3  | 8        | 0.21          |
| (2,1058) | 1:33:A:ILE:HB   | 1:22:A:ASN:HD22 | 3        | 0.21          |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG11 | 2        | 0.21          |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG12 | 2        | 0.21          |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG13 | 2        | 0.21          |
| (2,995)  | 1:13:A:MET:HB3  | 1:10:A:GLY:HA3  | 1        | 0.21          |
| (2,883)  | 1:81:A:ARG:HB3  | 1:80:A:SER:H    | 8        | 0.21          |
| (2,510)  | 1:19:A:ASP:HA   | 1:18:A:MET:HA   | 10       | 0.21          |
| (2,369)  | 1:19:A:ASP:HA   | 1:23:A:ASN:HB3  | 6        | 0.21          |
| (2,330)  | 1:48:A:LYS:HD3  | 1:93:A:GLU:HB2  | 2        | 0.21          |
| (2,271)  | 1:50:A:PHE:HA   | 1:51:A:LEU:H    | 4        | 0.21          |
| (2,234)  | 1:49:A:VAL:HG21 | 1:35:A:ILE:HA   | 2        | 0.21          |
| (2,234)  | 1:49:A:VAL:HG22 | 1:35:A:ILE:HA   | 2        | 0.21          |
| (2,234)  | 1:49:A:VAL:HG23 | 1:35:A:ILE:HA   | 2        | 0.21          |
| (2,208)  | 1:79:A:GLY:HA2  | 1:76:A:SER:HA   | 5        | 0.21          |
| (2,208)  | 1:79:A:GLY:HA2  | 1:76:A:SER:HA   | 7        | 0.21          |
| (2,192)  | 1:25:A:VAL:HG21 | 1:74:A:ILE:HA   | 10       | 0.21          |
| (2,192)  | 1:25:A:VAL:HG22 | 1:74:A:ILE:HA   | 10       | 0.21          |
| (2,192)  | 1:25:A:VAL:HG23 | 1:74:A:ILE:HA   | 10       | 0.21          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG21 | 1        | 0.21          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG22 | 1        | 0.21          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG23 | 1        | 0.21          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB1  | 4        | 0.21          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB2  | 4        | 0.21          |
| (2,156)  | 1:25:A:VAL:HG21 | 1:66:A:ALA:HB3  | 4        | 0.21          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB1  | 4        | 0.21          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB2  | 4        | 0.21          |
| (2,156)  | 1:25:A:VAL:HG22 | 1:66:A:ALA:HB3  | 4        | 0.21          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB1  | 4        | 0.21          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB2  | 4        | 0.21          |
| (2,156)  | 1:25:A:VAL:HG23 | 1:66:A:ALA:HB3  | 4        | 0.21          |
| (2,25)   | 1:15:A:LYS:C    | 1:19:A:ASP:H    | 2        | 0.21          |
| (2,20)   | 1:12:A:GLN:C    | 1:16:A:GLU:N    | 1        | 0.21          |
| (2,2991) | 1:98:A:ILE:H    | 1:99:A:GLU:HA   | 3        | 0.2           |
| (2,2913) | 1:77:A:GLU:H    | 1:78:A:LEU:HB2  | 2        | 0.2           |
| (2,2752) | 1:46:A:GLN:HE22 | 1:46:A:GLN:HA   | 6        | 0.2           |
| (2,2464) | 1:66:A:ALA:H    | 1:65:A:LYS:HG2  | 9        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2268) | 1:17:A:LEU:H    | 1:15:A:LYS:HB2  | 1        | 0.2           |
| (2,2268) | 1:17:A:LEU:H    | 1:15:A:LYS:HB2  | 9        | 0.2           |
| (2,2124) | 1:117:A:VAL:H   | 1:117:A:VAL:HB  | 7        | 0.2           |
| (2,1997) | 1:63:A:THR:H    | 1:62:A:ASN:HA   | 10       | 0.2           |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG21 | 1        | 0.2           |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG22 | 1        | 0.2           |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG23 | 1        | 0.2           |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG21 | 7        | 0.2           |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG22 | 7        | 0.2           |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG23 | 7        | 0.2           |
| (2,1849) | 1:21:A:ILE:H    | 1:25:A:VAL:HB   | 5        | 0.2           |
| (2,1814) | 1:14:A:LYS:H    | 1:12:A:GLN:HB2  | 1        | 0.2           |
| (2,1814) | 1:14:A:LYS:H    | 1:12:A:GLN:HB2  | 8        | 0.2           |
| (2,1353) | 1:92:A:TYR:HB3  | 1:64:A:PHE:HB3  | 10       | 0.2           |
| (2,1313) | 1:81:A:ARG:HB3  | 1:16:A:GLU:HB2  | 3        | 0.2           |
| (2,1247) | 1:68:A:ASP:HB2  | 1:71:A:LYS:HG3  | 7        | 0.2           |
| (2,1199) | 1:59:A:GLU:HB2  | 1:56:A:ASN:HD22 | 6        | 0.2           |
| (2,1058) | 1:33:A:ILE:HB   | 1:22:A:ASN:HD22 | 1        | 0.2           |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG11 | 3        | 0.2           |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG12 | 3        | 0.2           |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG13 | 3        | 0.2           |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG11 | 7        | 0.2           |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG12 | 7        | 0.2           |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG13 | 7        | 0.2           |
| (2,1002) | 1:16:A:GLU:HB2  | 1:81:A:ARG:HB3  | 3        | 0.2           |
| (2,995)  | 1:13:A:MET:HB3  | 1:10:A:GLY:HA3  | 3        | 0.2           |
| (2,507)  | 1:19:A:ASP:HA   | 1:22:A:ASN:HB3  | 6        | 0.2           |
| (2,507)  | 1:19:A:ASP:HA   | 1:22:A:ASN:HB3  | 10       | 0.2           |
| (2,437)  | 1:6:A:ALA:HB1   | 1:39:A:VAL:HG21 | 9        | 0.2           |
| (2,437)  | 1:6:A:ALA:HB1   | 1:39:A:VAL:HG22 | 9        | 0.2           |
| (2,437)  | 1:6:A:ALA:HB1   | 1:39:A:VAL:HG23 | 9        | 0.2           |
| (2,437)  | 1:6:A:ALA:HB2   | 1:39:A:VAL:HG21 | 9        | 0.2           |
| (2,437)  | 1:6:A:ALA:HB2   | 1:39:A:VAL:HG22 | 9        | 0.2           |
| (2,437)  | 1:6:A:ALA:HB2   | 1:39:A:VAL:HG23 | 9        | 0.2           |
| (2,437)  | 1:6:A:ALA:HB3   | 1:39:A:VAL:HG21 | 9        | 0.2           |
| (2,437)  | 1:6:A:ALA:HB3   | 1:39:A:VAL:HG22 | 9        | 0.2           |
| (2,437)  | 1:6:A:ALA:HB3   | 1:39:A:VAL:HG23 | 9        | 0.2           |
| (2,369)  | 1:19:A:ASP:HA   | 1:23:A:ASN:HB3  | 1        | 0.2           |
| (2,369)  | 1:19:A:ASP:HA   | 1:23:A:ASN:HB3  | 5        | 0.2           |
| (2,330)  | 1:48:A:LYS:HD3  | 1:93:A:GLU:HB2  | 9        | 0.2           |
| (2,318)  | 1:46:A:GLN:HG2  | 1:89:A:GLU:HB3  | 3        | 0.2           |
| (2,234)  | 1:49:A:VAL:HG21 | 1:35:A:ILE:HA   | 3        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,234)  | 1:49:A:VAL:HG22 | 1:35:A:ILE:HA   | 3        | 0.2           |
| (2,234)  | 1:49:A:VAL:HG23 | 1:35:A:ILE:HA   | 3        | 0.2           |
| (2,215)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB3  | 9        | 0.2           |
| (2,215)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB3  | 9        | 0.2           |
| (2,215)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB3  | 9        | 0.2           |
| (2,208)  | 1:79:A:GLY:HA2  | 1:76:A:SER:HA   | 9        | 0.2           |
| (2,192)  | 1:25:A:VAL:HG21 | 1:74:A:ILE:HA   | 5        | 0.2           |
| (2,192)  | 1:25:A:VAL:HG22 | 1:74:A:ILE:HA   | 5        | 0.2           |
| (2,192)  | 1:25:A:VAL:HG23 | 1:74:A:ILE:HA   | 5        | 0.2           |
| (2,125)  | 1:49:A:VAL:H    | 1:92:A:TYR:HA   | 9        | 0.2           |
| (2,26)   | 1:15:A:LYS:C    | 1:19:A:ASP:N    | 2        | 0.2           |
| (2,11)   | 1:8:A:ARG:C     | 1:12:A:GLN:H    | 5        | 0.2           |
| (1,150)  | 1:66:A:ALA:O    | 1:70:A:ALA:H    | 3        | 0.2           |
| (1,127)  | 1:20:A:ILE:O    | 1:24:A:LYS:H    | 3        | 0.2           |
| (2,3006) | 1:101:A:GLY:H   | 1:100:A:TYR:HA  | 4        | 0.19          |
| (2,2959) | 1:91:A:MET:H    | 1:47:A:ALA:HA   | 2        | 0.19          |
| (2,2912) | 1:76:A:SER:H    | 1:77:A:GLU:HB3  | 7        | 0.19          |
| (2,2886) | 1:71:A:LYS:H    | 1:69:A:LYS:HB3  | 1        | 0.19          |
| (2,2856) | 1:63:A:THR:H    | 1:65:A:LYS:HG2  | 4        | 0.19          |
| (2,2772) | 1:49:A:VAL:H    | 1:38:A:VAL:HG21 | 3        | 0.19          |
| (2,2772) | 1:49:A:VAL:H    | 1:38:A:VAL:HG22 | 3        | 0.19          |
| (2,2772) | 1:49:A:VAL:H    | 1:38:A:VAL:HG23 | 3        | 0.19          |
| (2,2758) | 1:47:A:ALA:H    | 1:89:A:GLU:HB3  | 10       | 0.19          |
| (2,2650) | 1:22:A:ASN:H    | 1:18:A:MET:HA   | 4        | 0.19          |
| (2,2650) | 1:22:A:ASN:H    | 1:18:A:MET:HA   | 10       | 0.19          |
| (2,2428) | 1:58:A:LYS:H    | 1:56:A:ASN:HA   | 4        | 0.19          |
| (2,2214) | 1:76:A:SER:H    | 1:78:A:LEU:HB2  | 8        | 0.19          |
| (2,2088) | 1:99:A:GLU:H    | 1:98:A:ILE:HG13 | 7        | 0.19          |
| (2,2088) | 1:99:A:GLU:H    | 1:98:A:ILE:HG13 | 9        | 0.19          |
| (2,2062) | 1:91:A:MET:H    | 1:49:A:VAL:HB   | 4        | 0.19          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG21 | 9        | 0.19          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG22 | 9        | 0.19          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG23 | 9        | 0.19          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG21 | 2        | 0.19          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG22 | 2        | 0.19          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG23 | 2        | 0.19          |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG21 | 9        | 0.19          |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG22 | 9        | 0.19          |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG23 | 9        | 0.19          |
| (2,1876) | 1:34:A:THR:H    | 1:52:A:THR:HB   | 6        | 0.19          |
| (2,1849) | 1:21:A:ILE:H    | 1:25:A:VAL:HB   | 6        | 0.19          |
| (2,1814) | 1:14:A:LYS:H    | 1:12:A:GLN:HB2  | 6        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1814) | 1:14:A:LYS:H    | 1:12:A:GLN:HB2  | 9        | 0.19          |
| (2,1781) | 1:22:A:ASN:HD22 | 1:22:A:ASN:HA   | 2        | 0.19          |
| (2,1106) | 1:39:A:VAL:HG21 | 1:48:A:LYS:HB3  | 9        | 0.19          |
| (2,1106) | 1:39:A:VAL:HG22 | 1:48:A:LYS:HB3  | 9        | 0.19          |
| (2,1106) | 1:39:A:VAL:HG23 | 1:48:A:LYS:HB3  | 9        | 0.19          |
| (2,997)  | 1:14:A:LYS:HA   | 1:17:A:LEU:HD21 | 2        | 0.19          |
| (2,997)  | 1:14:A:LYS:HA   | 1:17:A:LEU:HD22 | 2        | 0.19          |
| (2,997)  | 1:14:A:LYS:HA   | 1:17:A:LEU:HD23 | 2        | 0.19          |
| (2,919)  | 1:108:A:ILE:HA  | 1:110:A:ASP:HB2 | 7        | 0.19          |
| (2,601)  | 1:38:A:VAL:HG21 | 1:48:A:LYS:H    | 5        | 0.19          |
| (2,601)  | 1:38:A:VAL:HG22 | 1:48:A:LYS:H    | 5        | 0.19          |
| (2,601)  | 1:38:A:VAL:HG23 | 1:48:A:LYS:H    | 5        | 0.19          |
| (2,507)  | 1:19:A:ASP:HA   | 1:22:A:ASN:HB3  | 4        | 0.19          |
| (2,507)  | 1:19:A:ASP:HA   | 1:22:A:ASN:HB3  | 5        | 0.19          |
| (2,507)  | 1:19:A:ASP:HA   | 1:22:A:ASN:HB3  | 8        | 0.19          |
| (2,437)  | 1:6:A:ALA:HB1   | 1:39:A:VAL:HG21 | 3        | 0.19          |
| (2,437)  | 1:6:A:ALA:HB1   | 1:39:A:VAL:HG22 | 3        | 0.19          |
| (2,437)  | 1:6:A:ALA:HB1   | 1:39:A:VAL:HG23 | 3        | 0.19          |
| (2,437)  | 1:6:A:ALA:HB2   | 1:39:A:VAL:HG21 | 3        | 0.19          |
| (2,437)  | 1:6:A:ALA:HB2   | 1:39:A:VAL:HG22 | 3        | 0.19          |
| (2,437)  | 1:6:A:ALA:HB2   | 1:39:A:VAL:HG23 | 3        | 0.19          |
| (2,437)  | 1:6:A:ALA:HB3   | 1:39:A:VAL:HG21 | 3        | 0.19          |
| (2,437)  | 1:6:A:ALA:HB3   | 1:39:A:VAL:HG22 | 3        | 0.19          |
| (2,437)  | 1:6:A:ALA:HB3   | 1:39:A:VAL:HG23 | 3        | 0.19          |
| (2,369)  | 1:19:A:ASP:HA   | 1:23:A:ASN:HB3  | 9        | 0.19          |
| (2,238)  | 1:95:A:ASP:HA   | 1:50:A:PHE:HD1  | 8        | 0.19          |
| (2,238)  | 1:95:A:ASP:HA   | 1:50:A:PHE:HD2  | 8        | 0.19          |
| (2,234)  | 1:49:A:VAL:HG21 | 1:35:A:ILE:HA   | 1        | 0.19          |
| (2,234)  | 1:49:A:VAL:HG22 | 1:35:A:ILE:HA   | 1        | 0.19          |
| (2,234)  | 1:49:A:VAL:HG23 | 1:35:A:ILE:HA   | 1        | 0.19          |
| (2,216)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB2  | 7        | 0.19          |
| (2,216)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB2  | 7        | 0.19          |
| (2,216)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB2  | 7        | 0.19          |
| (2,121)  | 1:45:A:SER:HA   | 1:88:A:PRO:HA   | 2        | 0.19          |
| (2,120)  | 1:33:A:ILE:HA   | 1:53:A:VAL:HA   | 3        | 0.19          |
| (2,120)  | 1:33:A:ILE:HA   | 1:53:A:VAL:HA   | 10       | 0.19          |
| (2,20)   | 1:12:A:GLN:C    | 1:16:A:GLU:N    | 5        | 0.19          |
| (2,19)   | 1:12:A:GLN:C    | 1:16:A:GLU:H    | 4        | 0.19          |
| (1,143)  | 1:76:A:SER:O    | 1:80:A:SER:H    | 3        | 0.19          |
| (1,128)  | 1:21:A:ILE:O    | 1:25:A:VAL:H    | 4        | 0.19          |
| (2,2991) | 1:98:A:ILE:H    | 1:99:A:GLU:HA   | 1        | 0.18          |
| (2,2991) | 1:98:A:ILE:H    | 1:99:A:GLU:HA   | 6        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2899) | 1:74:A:ILE:H    | 1:71:A:LYS:HB3  | 8        | 0.18          |
| (2,2881) | 1:70:A:ALA:H    | 1:71:A:LYS:HB3  | 8        | 0.18          |
| (2,2772) | 1:49:A:VAL:H    | 1:38:A:VAL:HG21 | 6        | 0.18          |
| (2,2772) | 1:49:A:VAL:H    | 1:38:A:VAL:HG22 | 6        | 0.18          |
| (2,2772) | 1:49:A:VAL:H    | 1:38:A:VAL:HG23 | 6        | 0.18          |
| (2,2741) | 1:44:A:LEU:H    | 1:45:A:SER:HB3  | 8        | 0.18          |
| (2,2681) | 1:34:A:THR:H    | 1:51:A:LEU:HB2  | 4        | 0.18          |
| (2,2657) | 1:23:A:ASN:H    | 1:23:A:ASN:HD22 | 3        | 0.18          |
| (2,2650) | 1:22:A:ASN:H    | 1:18:A:MET:HA   | 6        | 0.18          |
| (2,2650) | 1:22:A:ASN:H    | 1:18:A:MET:HA   | 7        | 0.18          |
| (2,2464) | 1:66:A:ALA:H    | 1:65:A:LYS:HG2  | 5        | 0.18          |
| (2,2464) | 1:66:A:ALA:H    | 1:65:A:LYS:HG2  | 6        | 0.18          |
| (2,2428) | 1:58:A:LYS:H    | 1:56:A:ASN:HA   | 2        | 0.18          |
| (2,2088) | 1:99:A:GLU:H    | 1:98:A:ILE:HG13 | 3        | 0.18          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG21 | 2        | 0.18          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG22 | 2        | 0.18          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG23 | 2        | 0.18          |
| (2,1814) | 1:14:A:LYS:H    | 1:12:A:GLN:HB2  | 2        | 0.18          |
| (2,1617) | 1:66:A:ALA:H    | 1:69:A:LYS:HB3  | 4        | 0.18          |
| (2,1616) | 1:66:A:ALA:H    | 1:65:A:LYS:HD2  | 4        | 0.18          |
| (2,1495) | 1:46:A:GLN:H    | 1:45:A:SER:H    | 10       | 0.18          |
| (2,960)  | 1:118:A:GLU:HA  | 1:117:A:VAL:HB  | 2        | 0.18          |
| (2,941)  | 1:111:A:LEU:HA  | 1:110:A:ASP:H   | 2        | 0.18          |
| (2,941)  | 1:111:A:LEU:HA  | 1:110:A:ASP:H   | 3        | 0.18          |
| (2,938)  | 1:111:A:LEU:HA  | 1:113:A:LYS:HB3 | 8        | 0.18          |
| (2,919)  | 1:108:A:ILE:HA  | 1:110:A:ASP:HB2 | 9        | 0.18          |
| (2,785)  | 1:65:A:LYS:HD2  | 1:65:A:LYS:HA   | 4        | 0.18          |
| (2,369)  | 1:19:A:ASP:HA   | 1:23:A:ASN:HB3  | 3        | 0.18          |
| (2,334)  | 1:17:A:LEU:HD21 | 1:13:A:MET:HB3  | 5        | 0.18          |
| (2,334)  | 1:17:A:LEU:HD22 | 1:13:A:MET:HB3  | 5        | 0.18          |
| (2,334)  | 1:17:A:LEU:HD23 | 1:13:A:MET:HB3  | 5        | 0.18          |
| (2,270)  | 1:47:A:ALA:HA   | 1:40:A:LEU:HA   | 8        | 0.18          |
| (2,208)  | 1:79:A:GLY:HA2  | 1:76:A:SER:HA   | 8        | 0.18          |
| (2,136)  | 1:31:A:GLY:HA2  | 1:54:A:LEU:HB3  | 4        | 0.18          |
| (2,136)  | 1:31:A:GLY:HA2  | 1:54:A:LEU:HB3  | 8        | 0.18          |
| (2,136)  | 1:31:A:GLY:HA2  | 1:54:A:LEU:HB3  | 9        | 0.18          |
| (2,31)   | 1:18:A:MET:C    | 1:22:A:ASN:H    | 1        | 0.18          |
| (2,13)   | 1:9:A:VAL:C     | 1:13:A:MET:H    | 4        | 0.18          |
| (2,11)   | 1:8:A:ARG:C     | 1:12:A:GLN:H    | 8        | 0.18          |
| (1,143)  | 1:76:A:SER:O    | 1:80:A:SER:H    | 7        | 0.18          |
| (1,127)  | 1:20:A:ILE:O    | 1:24:A:LYS:H    | 4        | 0.18          |
| (1,116)  | 1:9:A:VAL:O     | 1:13:A:MET:H    | 7        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,46)   | 1:65:A:LYS:H    | 1:61:A:GLU:O    | 1        | 0.18          |
| (2,2975) | 1:96:A:GLN:H    | 1:96:A:GLN:HE22 | 8        | 0.17          |
| (2,2804) | 1:56:A:ASN:HD22 | 1:56:A:ASN:HA   | 6        | 0.17          |
| (2,2752) | 1:46:A:GLN:HE22 | 1:46:A:GLN:HA   | 10       | 0.17          |
| (2,2681) | 1:34:A:THR:H    | 1:51:A:LEU:HB2  | 9        | 0.17          |
| (2,2657) | 1:23:A:ASN:H    | 1:23:A:ASN:HD22 | 4        | 0.17          |
| (2,2464) | 1:66:A:ALA:H    | 1:65:A:LYS:HG2  | 2        | 0.17          |
| (2,2464) | 1:66:A:ALA:H    | 1:65:A:LYS:HG2  | 4        | 0.17          |
| (2,2428) | 1:58:A:LYS:H    | 1:56:A:ASN:HA   | 3        | 0.17          |
| (2,2428) | 1:58:A:LYS:H    | 1:56:A:ASN:HA   | 9        | 0.17          |
| (2,2214) | 1:76:A:SER:H    | 1:78:A:LEU:HB2  | 1        | 0.17          |
| (2,2124) | 1:117:A:VAL:H   | 1:117:A:VAL:HB  | 5        | 0.17          |
| (2,2088) | 1:99:A:GLU:H    | 1:98:A:ILE:HG13 | 2        | 0.17          |
| (2,2038) | 1:76:A:SER:H    | 1:72:A:GLY:HA3  | 5        | 0.17          |
| (2,1992) | 1:64:A:PHE:H    | 1:62:A:ASN:HB2  | 3        | 0.17          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG21 | 7        | 0.17          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG22 | 7        | 0.17          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG23 | 7        | 0.17          |
| (2,1886) | 1:36:A:THR:H    | 1:37:A:ASP:HA   | 9        | 0.17          |
| (2,1814) | 1:14:A:LYS:H    | 1:12:A:GLN:HB2  | 7        | 0.17          |
| (2,1617) | 1:66:A:ALA:H    | 1:69:A:LYS:HB3  | 5        | 0.17          |
| (2,1599) | 1:62:A:ASN:H    | 1:64:A:PHE:HB3  | 1        | 0.17          |
| (2,1575) | 1:58:A:LYS:H    | 1:59:A:GLU:HG3  | 9        | 0.17          |
| (2,1344) | 1:98:A:ILE:HG12 | 1:95:A:ASP:HB2  | 8        | 0.17          |
| (2,1344) | 1:98:A:ILE:HG12 | 1:95:A:ASP:HB2  | 10       | 0.17          |
| (2,1199) | 1:59:A:GLU:HB2  | 1:56:A:ASN:HD22 | 10       | 0.17          |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG11 | 1        | 0.17          |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG12 | 1        | 0.17          |
| (2,1028) | 1:24:A:LYS:HB3  | 1:25:A:VAL:HG13 | 1        | 0.17          |
| (2,941)  | 1:111:A:LEU:HA  | 1:110:A:ASP:H   | 5        | 0.17          |
| (2,934)  | 1:109:A:GLN:HB2 | 1:110:A:ASP:HB2 | 1        | 0.17          |
| (2,932)  | 1:109:A:GLN:HB2 | 1:107:A:MET:HA  | 3        | 0.17          |
| (2,883)  | 1:81:A:ARG:HB3  | 1:80:A:SER:H    | 4        | 0.17          |
| (2,785)  | 1:65:A:LYS:HD2  | 1:65:A:LYS:HA   | 3        | 0.17          |
| (2,585)  | 1:37:A:ASP:HA   | 1:38:A:VAL:H    | 5        | 0.17          |
| (2,510)  | 1:19:A:ASP:HA   | 1:18:A:MET:HA   | 9        | 0.17          |
| (2,507)  | 1:19:A:ASP:HA   | 1:22:A:ASN:HB3  | 9        | 0.17          |
| (2,265)  | 1:44:A:LEU:H    | 1:43:A:ASP:H    | 8        | 0.17          |
| (2,238)  | 1:95:A:ASP:HA   | 1:50:A:PHE:HD1  | 7        | 0.17          |
| (2,238)  | 1:95:A:ASP:HA   | 1:50:A:PHE:HD2  | 7        | 0.17          |
| (2,192)  | 1:25:A:VAL:HG21 | 1:74:A:ILE:HA   | 6        | 0.17          |
| (2,192)  | 1:25:A:VAL:HG22 | 1:74:A:ILE:HA   | 6        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,192)  | 1:25:A:VAL:HG23 | 1:74:A:ILE:HA   | 6        | 0.17          |
| (2,126)  | 1:93:A:GLU:H    | 1:50:A:PHE:HA   | 4        | 0.17          |
| (2,121)  | 1:45:A:SER:HA   | 1:88:A:PRO:HA   | 6        | 0.17          |
| (2,93)   | 1:60:A:VAL:C    | 1:64:A:PHE:H    | 9        | 0.17          |
| (2,87)   | 1:63:A:THR:C    | 1:67:A:LEU:H    | 8        | 0.17          |
| (2,87)   | 1:63:A:THR:C    | 1:67:A:LEU:H    | 9        | 0.17          |
| (2,20)   | 1:12:A:GLN:C    | 1:16:A:GLU:N    | 4        | 0.17          |
| (2,17)   | 1:11:A:GLU:C    | 1:15:A:LYS:H    | 6        | 0.17          |
| (2,12)   | 1:8:A:ARG:C     | 1:12:A:GLN:N    | 5        | 0.17          |
| (2,5)    | 1:5:A:ARG:C     | 1:9:A:VAL:H     | 6        | 0.17          |
| (1,46)   | 1:65:A:LYS:H    | 1:61:A:GLU:O    | 2        | 0.17          |
| (2,3006) | 1:101:A:GLY:H   | 1:100:A:TYR:HA  | 2        | 0.16          |
| (2,2991) | 1:98:A:ILE:H    | 1:99:A:GLU:HA   | 10       | 0.16          |
| (2,2913) | 1:77:A:GLU:H    | 1:78:A:LEU:HB2  | 6        | 0.16          |
| (2,2912) | 1:76:A:SER:H    | 1:77:A:GLU:HB3  | 3        | 0.16          |
| (2,2886) | 1:71:A:LYS:H    | 1:69:A:LYS:HB3  | 4        | 0.16          |
| (2,2886) | 1:71:A:LYS:H    | 1:69:A:LYS:HB3  | 8        | 0.16          |
| (2,2881) | 1:70:A:ALA:H    | 1:71:A:LYS:HB3  | 2        | 0.16          |
| (2,2772) | 1:49:A:VAL:H    | 1:38:A:VAL:HG21 | 1        | 0.16          |
| (2,2772) | 1:49:A:VAL:H    | 1:38:A:VAL:HG22 | 1        | 0.16          |
| (2,2772) | 1:49:A:VAL:H    | 1:38:A:VAL:HG23 | 1        | 0.16          |
| (2,2650) | 1:22:A:ASN:H    | 1:18:A:MET:HA   | 5        | 0.16          |
| (2,2268) | 1:17:A:LEU:H    | 1:15:A:LYS:HB2  | 10       | 0.16          |
| (2,2062) | 1:91:A:MET:H    | 1:49:A:VAL:HB   | 5        | 0.16          |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG21 | 2        | 0.16          |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG22 | 2        | 0.16          |
| (2,1891) | 1:36:A:THR:H    | 1:38:A:VAL:HG23 | 2        | 0.16          |
| (2,1823) | 1:15:A:LYS:H    | 1:18:A:MET:HB2  | 8        | 0.16          |
| (2,1822) | 1:15:A:LYS:H    | 1:12:A:GLN:HB2  | 6        | 0.16          |
| (2,1701) | 1:79:A:GLY:H    | 1:75:A:LYS:HB3  | 9        | 0.16          |
| (2,1688) | 1:77:A:GLU:H    | 1:73:A:PHE:HA   | 5        | 0.16          |
| (2,1688) | 1:77:A:GLU:H    | 1:73:A:PHE:HA   | 6        | 0.16          |
| (2,1599) | 1:62:A:ASN:H    | 1:64:A:PHE:HB3  | 6        | 0.16          |
| (2,1575) | 1:58:A:LYS:H    | 1:59:A:GLU:HG3  | 10       | 0.16          |
| (2,1495) | 1:46:A:GLN:H    | 1:45:A:SER:H    | 3        | 0.16          |
| (2,1313) | 1:81:A:ARG:HB3  | 1:16:A:GLU:HB2  | 8        | 0.16          |
| (2,1247) | 1:68:A:ASP:HB2  | 1:71:A:LYS:HG3  | 4        | 0.16          |
| (2,1227) | 1:65:A:LYS:HG2  | 1:61:A:GLU:HB2  | 4        | 0.16          |
| (2,1216) | 1:62:A:ASN:HA   | 1:65:A:LYS:HD2  | 10       | 0.16          |
| (2,1199) | 1:59:A:GLU:HB2  | 1:56:A:ASN:HD22 | 3        | 0.16          |
| (2,1002) | 1:16:A:GLU:HB2  | 1:81:A:ARG:HB3  | 8        | 0.16          |
| (2,995)  | 1:13:A:MET:HB3  | 1:10:A:GLY:HA3  | 2        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,994) | 1:13:A:MET:HB3  | 1:38:A:VAL:HB   | 5        | 0.16          |
| (2,960) | 1:118:A:GLU:HA  | 1:117:A:VAL:HB  | 10       | 0.16          |
| (2,934) | 1:109:A:GLN:HB2 | 1:110:A:ASP:HB2 | 2        | 0.16          |
| (2,934) | 1:109:A:GLN:HB2 | 1:110:A:ASP:HB2 | 10       | 0.16          |
| (2,932) | 1:109:A:GLN:HB2 | 1:107:A:MET:HA  | 2        | 0.16          |
| (2,919) | 1:108:A:ILE:HA  | 1:110:A:ASP:HB2 | 4        | 0.16          |
| (2,785) | 1:65:A:LYS:HD2  | 1:65:A:LYS:HA   | 6        | 0.16          |
| (2,785) | 1:65:A:LYS:HD2  | 1:65:A:LYS:HA   | 9        | 0.16          |
| (2,604) | 1:38:A:VAL:HG21 | 1:47:A:ALA:HA   | 8        | 0.16          |
| (2,604) | 1:38:A:VAL:HG22 | 1:47:A:ALA:HA   | 8        | 0.16          |
| (2,604) | 1:38:A:VAL:HG23 | 1:47:A:ALA:HA   | 8        | 0.16          |
| (2,528) | 1:22:A:ASN:HA   | 1:33:A:ILE:HB   | 9        | 0.16          |
| (2,345) | 1:74:A:ILE:HB   | 1:71:A:LYS:HA   | 7        | 0.16          |
| (2,270) | 1:47:A:ALA:HA   | 1:40:A:LEU:HA   | 10       | 0.16          |
| (2,238) | 1:95:A:ASP:HA   | 1:50:A:PHE:HD1  | 3        | 0.16          |
| (2,238) | 1:95:A:ASP:HA   | 1:50:A:PHE:HD2  | 3        | 0.16          |
| (2,238) | 1:95:A:ASP:HA   | 1:50:A:PHE:HD1  | 4        | 0.16          |
| (2,238) | 1:95:A:ASP:HA   | 1:50:A:PHE:HD2  | 4        | 0.16          |
| (2,238) | 1:95:A:ASP:HA   | 1:50:A:PHE:HD1  | 9        | 0.16          |
| (2,238) | 1:95:A:ASP:HA   | 1:50:A:PHE:HD2  | 9        | 0.16          |
| (2,234) | 1:49:A:VAL:HG21 | 1:35:A:ILE:HA   | 5        | 0.16          |
| (2,234) | 1:49:A:VAL:HG22 | 1:35:A:ILE:HA   | 5        | 0.16          |
| (2,234) | 1:49:A:VAL:HG23 | 1:35:A:ILE:HA   | 5        | 0.16          |
| (2,120) | 1:33:A:ILE:HA   | 1:53:A:VAL:HA   | 5        | 0.16          |
| (2,120) | 1:33:A:ILE:HA   | 1:53:A:VAL:HA   | 8        | 0.16          |
| (2,87)  | 1:63:A:THR:C    | 1:67:A:LEU:H    | 2        | 0.16          |
| (2,87)  | 1:63:A:THR:C    | 1:67:A:LEU:H    | 10       | 0.16          |
| (2,79)  | 1:70:A:ALA:C    | 1:74:A:ILE:H    | 4        | 0.16          |
| (2,32)  | 1:18:A:MET:C    | 1:22:A:ASN:N    | 1        | 0.16          |
| (2,31)  | 1:18:A:MET:C    | 1:22:A:ASN:H    | 3        | 0.16          |
| (2,25)  | 1:15:A:LYS:C    | 1:19:A:ASP:H    | 4        | 0.16          |
| (2,19)  | 1:12:A:GLN:C    | 1:16:A:GLU:H    | 2        | 0.16          |
| (2,13)  | 1:9:A:VAL:C     | 1:13:A:MET:H    | 7        | 0.16          |
| (2,12)  | 1:8:A:ARG:C     | 1:12:A:GLN:N    | 8        | 0.16          |
| (2,6)   | 1:5:A:ARG:C     | 1:9:A:VAL:N     | 6        | 0.16          |
| (2,6)   | 1:5:A:ARG:C     | 1:9:A:VAL:N     | 7        | 0.16          |
| (2,5)   | 1:5:A:ARG:C     | 1:9:A:VAL:H     | 7        | 0.16          |
| (1,153) | 1:63:A:THR:O    | 1:67:A:LEU:H    | 2        | 0.16          |
| (1,127) | 1:20:A:ILE:O    | 1:24:A:LYS:H    | 10       | 0.16          |
| (1,122) | 1:15:A:LYS:O    | 1:19:A:ASP:H    | 7        | 0.16          |
| (1,118) | 1:11:A:GLU:O    | 1:15:A:LYS:H    | 1        | 0.16          |
| (1,117) | 1:10:A:GLY:O    | 1:14:A:LYS:H    | 6        | 0.16          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (1,116)  | 1:9:A:VAL:O  | 1:13:A:MET:H    | 2        | 0.16          |
| (1,116)  | 1:9:A:VAL:O  | 1:13:A:MET:H    | 6        | 0.16          |
| (1,46)   | 1:65:A:LYS:H | 1:61:A:GLU:O    | 6        | 0.16          |
| (1,46)   | 1:65:A:LYS:H | 1:61:A:GLU:O    | 9        | 0.16          |
| (2,2960) | 1:91:A:MET:H | 1:92:A:TYR:HA   | 9        | 0.15          |
| (2,2913) | 1:77:A:GLU:H | 1:78:A:LEU:HB2  | 7        | 0.15          |
| (2,2912) | 1:76:A:SER:H | 1:77:A:GLU:HB3  | 8        | 0.15          |
| (2,2899) | 1:74:A:ILE:H | 1:71:A:LYS:HB3  | 2        | 0.15          |
| (2,2886) | 1:71:A:LYS:H | 1:69:A:LYS:HB3  | 6        | 0.15          |
| (2,2886) | 1:71:A:LYS:H | 1:69:A:LYS:HB3  | 7        | 0.15          |
| (2,2772) | 1:49:A:VAL:H | 1:38:A:VAL:HG21 | 9        | 0.15          |
| (2,2772) | 1:49:A:VAL:H | 1:38:A:VAL:HG22 | 9        | 0.15          |
| (2,2772) | 1:49:A:VAL:H | 1:38:A:VAL:HG23 | 9        | 0.15          |
| (2,2743) | 1:45:A:SER:H | 1:46:A:GLN:HA   | 1        | 0.15          |
| (2,2743) | 1:45:A:SER:H | 1:46:A:GLN:HA   | 2        | 0.15          |
| (2,2692) | 1:35:A:ILE:H | 1:36:A:THR:HA   | 9        | 0.15          |
| (2,2681) | 1:34:A:THR:H | 1:51:A:LEU:HB2  | 6        | 0.15          |
| (2,2681) | 1:34:A:THR:H | 1:51:A:LEU:HB2  | 7        | 0.15          |
| (2,2657) | 1:23:A:ASN:H | 1:23:A:ASN:HD22 | 5        | 0.15          |
| (2,2268) | 1:17:A:LEU:H | 1:15:A:LYS:HB2  | 7        | 0.15          |
| (2,2090) | 1:99:A:GLU:H | 1:101:A:GLY:HA2 | 1        | 0.15          |
| (2,2038) | 1:76:A:SER:H | 1:72:A:GLY:HA3  | 1        | 0.15          |
| (2,2038) | 1:76:A:SER:H | 1:72:A:GLY:HA3  | 2        | 0.15          |
| (2,2014) | 1:68:A:ASP:H | 1:65:A:LYS:HB2  | 7        | 0.15          |
| (2,1917) | 1:41:A:THR:H | 1:39:A:VAL:HG21 | 4        | 0.15          |
| (2,1917) | 1:41:A:THR:H | 1:39:A:VAL:HG22 | 4        | 0.15          |
| (2,1917) | 1:41:A:THR:H | 1:39:A:VAL:HG23 | 4        | 0.15          |
| (2,1900) | 1:38:A:VAL:H | 1:39:A:VAL:HG21 | 5        | 0.15          |
| (2,1900) | 1:38:A:VAL:H | 1:39:A:VAL:HG22 | 5        | 0.15          |
| (2,1900) | 1:38:A:VAL:H | 1:39:A:VAL:HG23 | 5        | 0.15          |
| (2,1900) | 1:38:A:VAL:H | 1:39:A:VAL:HG21 | 7        | 0.15          |
| (2,1900) | 1:38:A:VAL:H | 1:39:A:VAL:HG22 | 7        | 0.15          |
| (2,1900) | 1:38:A:VAL:H | 1:39:A:VAL:HG23 | 7        | 0.15          |
| (2,1823) | 1:15:A:LYS:H | 1:18:A:MET:HB2  | 4        | 0.15          |
| (2,1746) | 1:99:A:GLU:H | 1:98:A:ILE:HD11 | 8        | 0.15          |
| (2,1746) | 1:99:A:GLU:H | 1:98:A:ILE:HD12 | 8        | 0.15          |
| (2,1746) | 1:99:A:GLU:H | 1:98:A:ILE:HD13 | 8        | 0.15          |
| (2,1688) | 1:77:A:GLU:H | 1:73:A:PHE:HA   | 3        | 0.15          |
| (2,1688) | 1:77:A:GLU:H | 1:73:A:PHE:HA   | 4        | 0.15          |
| (2,1686) | 1:76:A:SER:H | 1:75:A:LYS:HG2  | 4        | 0.15          |
| (2,1628) | 1:68:A:ASP:H | 1:69:A:LYS:HB3  | 7        | 0.15          |
| (2,1617) | 1:66:A:ALA:H | 1:69:A:LYS:HB3  | 2        | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1389) | 1:15:A:LYS:H    | 1:16:A:GLU:HB2   | 6        | 0.15          |
| (2,1344) | 1:98:A:ILE:HG12 | 1:95:A:ASP:HB2   | 9        | 0.15          |
| (2,1313) | 1:81:A:ARG:HB3  | 1:16:A:GLU:HB2   | 7        | 0.15          |
| (2,1092) | 1:38:A:VAL:HG21 | 1:17:A:LEU:HB3   | 10       | 0.15          |
| (2,1092) | 1:38:A:VAL:HG22 | 1:17:A:LEU:HB3   | 10       | 0.15          |
| (2,1092) | 1:38:A:VAL:HG23 | 1:17:A:LEU:HB3   | 10       | 0.15          |
| (2,1031) | 1:24:A:LYS:HB2  | 1:25:A:VAL:HG11  | 8        | 0.15          |
| (2,1031) | 1:24:A:LYS:HB2  | 1:25:A:VAL:HG12  | 8        | 0.15          |
| (2,1031) | 1:24:A:LYS:HB2  | 1:25:A:VAL:HG13  | 8        | 0.15          |
| (2,1002) | 1:16:A:GLU:HB2  | 1:81:A:ARG:HB3   | 7        | 0.15          |
| (2,994)  | 1:13:A:MET:HB3  | 1:38:A:VAL:HB    | 7        | 0.15          |
| (2,960)  | 1:118:A:GLU:HA  | 1:117:A:VAL:HB   | 6        | 0.15          |
| (2,931)  | 1:109:A:GLN:HB2 | 1:109:A:GLN:HE22 | 7        | 0.15          |
| (2,917)  | 1:108:A:ILE:HA  | 1:107:A:MET:HB2  | 8        | 0.15          |
| (2,883)  | 1:81:A:ARG:HB3  | 1:80:A:SER:H     | 1        | 0.15          |
| (2,848)  | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3   | 2        | 0.15          |
| (2,848)  | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3   | 10       | 0.15          |
| (2,785)  | 1:65:A:LYS:HD2  | 1:65:A:LYS:HA    | 5        | 0.15          |
| (2,510)  | 1:19:A:ASP:HA   | 1:18:A:MET:HA    | 7        | 0.15          |
| (2,457)  | 1:11:A:GLU:HA   | 1:38:A:VAL:HB    | 10       | 0.15          |
| (2,334)  | 1:17:A:LEU:HD21 | 1:13:A:MET:HB3   | 4        | 0.15          |
| (2,334)  | 1:17:A:LEU:HD22 | 1:13:A:MET:HB3   | 4        | 0.15          |
| (2,334)  | 1:17:A:LEU:HD23 | 1:13:A:MET:HB3   | 4        | 0.15          |
| (2,281)  | 1:10:A:GLY:HA2  | 1:38:A:VAL:HB    | 3        | 0.15          |
| (2,239)  | 1:50:A:PHE:HB3  | 1:95:A:ASP:HA    | 9        | 0.15          |
| (2,208)  | 1:79:A:GLY:HA2  | 1:76:A:SER:HA    | 10       | 0.15          |
| (2,192)  | 1:25:A:VAL:HG21 | 1:74:A:ILE:HA    | 2        | 0.15          |
| (2,192)  | 1:25:A:VAL:HG22 | 1:74:A:ILE:HA    | 2        | 0.15          |
| (2,192)  | 1:25:A:VAL:HG23 | 1:74:A:ILE:HA    | 2        | 0.15          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG21  | 7        | 0.15          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG22  | 7        | 0.15          |
| (2,191)  | 1:74:A:ILE:HA   | 1:25:A:VAL:HG23  | 7        | 0.15          |
| (2,175)  | 1:72:A:GLY:HA3  | 1:75:A:LYS:HB3   | 2        | 0.15          |
| (2,175)  | 1:72:A:GLY:HA3  | 1:75:A:LYS:HB3   | 10       | 0.15          |
| (2,120)  | 1:33:A:ILE:HA   | 1:53:A:VAL:HA    | 1        | 0.15          |
| (2,94)   | 1:60:A:VAL:C    | 1:64:A:PHE:N     | 9        | 0.15          |
| (2,93)   | 1:60:A:VAL:C    | 1:64:A:PHE:H     | 1        | 0.15          |
| (2,93)   | 1:60:A:VAL:C    | 1:64:A:PHE:H     | 2        | 0.15          |
| (2,87)   | 1:63:A:THR:C    | 1:67:A:LEU:H     | 3        | 0.15          |
| (2,87)   | 1:63:A:THR:C    | 1:67:A:LEU:H     | 7        | 0.15          |
| (2,80)   | 1:70:A:ALA:C    | 1:74:A:ILE:N     | 4        | 0.15          |
| (2,73)   | 1:73:A:PHE:C    | 1:77:A:GLU:H     | 10       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,31)   | 1:18:A:MET:C    | 1:22:A:ASN:H    | 6        | 0.15          |
| (2,31)   | 1:18:A:MET:C    | 1:22:A:ASN:H    | 7        | 0.15          |
| (2,31)   | 1:18:A:MET:C    | 1:22:A:ASN:H    | 10       | 0.15          |
| (2,26)   | 1:15:A:LYS:C    | 1:19:A:ASP:N    | 4        | 0.15          |
| (2,25)   | 1:15:A:LYS:C    | 1:19:A:ASP:H    | 9        | 0.15          |
| (2,19)   | 1:12:A:GLN:C    | 1:16:A:GLU:H    | 8        | 0.15          |
| (2,14)   | 1:9:A:VAL:C     | 1:13:A:MET:N    | 4        | 0.15          |
| (2,11)   | 1:8:A:ARG:C     | 1:12:A:GLN:H    | 10       | 0.15          |
| (1,153)  | 1:63:A:THR:O    | 1:67:A:LEU:H    | 1        | 0.15          |
| (1,150)  | 1:66:A:ALA:O    | 1:70:A:ALA:H    | 4        | 0.15          |
| (1,150)  | 1:66:A:ALA:O    | 1:70:A:ALA:H    | 9        | 0.15          |
| (1,150)  | 1:66:A:ALA:O    | 1:70:A:ALA:H    | 10       | 0.15          |
| (1,143)  | 1:76:A:SER:O    | 1:80:A:SER:H    | 4        | 0.15          |
| (1,128)  | 1:21:A:ILE:O    | 1:25:A:VAL:H    | 10       | 0.15          |
| (1,127)  | 1:20:A:ILE:O    | 1:24:A:LYS:H    | 2        | 0.15          |
| (1,117)  | 1:10:A:GLY:O    | 1:14:A:LYS:H    | 9        | 0.15          |
| (1,115)  | 1:8:A:ARG:O     | 1:12:A:GLN:H    | 9        | 0.15          |
| (1,114)  | 1:7:A:GLU:O     | 1:11:A:GLU:H    | 5        | 0.15          |
| (1,46)   | 1:65:A:LYS:H    | 1:61:A:GLU:O    | 3        | 0.15          |
| (1,42)   | 1:69:A:LYS:H    | 1:65:A:LYS:O    | 3        | 0.15          |
| (2,2991) | 1:98:A:ILE:H    | 1:99:A:GLU:HA   | 7        | 0.14          |
| (2,2913) | 1:77:A:GLU:H    | 1:78:A:LEU:HB2  | 10       | 0.14          |
| (2,2912) | 1:76:A:SER:H    | 1:77:A:GLU:HB3  | 4        | 0.14          |
| (2,2856) | 1:63:A:THR:H    | 1:65:A:LYS:HG2  | 2        | 0.14          |
| (2,2819) | 1:58:A:LYS:H    | 1:59:A:GLU:HB2  | 2        | 0.14          |
| (2,2804) | 1:56:A:ASN:HD22 | 1:56:A:ASN:HA   | 7        | 0.14          |
| (2,2737) | 1:43:A:ASP:H    | 1:45:A:SER:HB3  | 1        | 0.14          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG21 | 10       | 0.14          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG22 | 10       | 0.14          |
| (2,2706) | 1:37:A:ASP:H    | 1:49:A:VAL:HG23 | 10       | 0.14          |
| (2,2681) | 1:34:A:THR:H    | 1:51:A:LEU:HB2  | 3        | 0.14          |
| (2,2657) | 1:23:A:ASN:H    | 1:23:A:ASN:HD22 | 9        | 0.14          |
| (2,2428) | 1:58:A:LYS:H    | 1:56:A:ASN:HA   | 10       | 0.14          |
| (2,2268) | 1:17:A:LEU:H    | 1:15:A:LYS:HB2  | 5        | 0.14          |
| (2,2214) | 1:76:A:SER:H    | 1:78:A:LEU:HB2  | 2        | 0.14          |
| (2,2096) | 1:102:A:ASN:H   | 1:101:A:GLY:HA2 | 5        | 0.14          |
| (2,2096) | 1:102:A:ASN:H   | 1:101:A:GLY:HA2 | 7        | 0.14          |
| (2,2088) | 1:99:A:GLU:H    | 1:98:A:ILE:HG13 | 6        | 0.14          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG21 | 5        | 0.14          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG22 | 5        | 0.14          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG23 | 5        | 0.14          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG21 | 10       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG22 | 10       | 0.14          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG23 | 10       | 0.14          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG21 | 7        | 0.14          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG22 | 7        | 0.14          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG23 | 7        | 0.14          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG21 | 4        | 0.14          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG22 | 4        | 0.14          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG23 | 4        | 0.14          |
| (2,1688) | 1:77:A:GLU:H    | 1:73:A:PHE:HA   | 2        | 0.14          |
| (2,1688) | 1:77:A:GLU:H    | 1:73:A:PHE:HA   | 10       | 0.14          |
| (2,1617) | 1:66:A:ALA:H    | 1:69:A:LYS:HB3  | 10       | 0.14          |
| (2,1599) | 1:62:A:ASN:H    | 1:64:A:PHE:HB3  | 3        | 0.14          |
| (2,1495) | 1:46:A:GLN:H    | 1:45:A:SER:H    | 4        | 0.14          |
| (2,1216) | 1:62:A:ASN:HA   | 1:65:A:LYS:HD2  | 8        | 0.14          |
| (2,1199) | 1:59:A:GLU:HB2  | 1:56:A:ASN:HD22 | 1        | 0.14          |
| (2,1199) | 1:59:A:GLU:HB2  | 1:56:A:ASN:HD22 | 4        | 0.14          |
| (2,1158) | 1:52:A:THR:HG21 | 1:36:A:THR:HG21 | 8        | 0.14          |
| (2,1158) | 1:52:A:THR:HG21 | 1:36:A:THR:HG22 | 8        | 0.14          |
| (2,1158) | 1:52:A:THR:HG21 | 1:36:A:THR:HG23 | 8        | 0.14          |
| (2,1158) | 1:52:A:THR:HG22 | 1:36:A:THR:HG21 | 8        | 0.14          |
| (2,1158) | 1:52:A:THR:HG22 | 1:36:A:THR:HG22 | 8        | 0.14          |
| (2,1158) | 1:52:A:THR:HG22 | 1:36:A:THR:HG23 | 8        | 0.14          |
| (2,1158) | 1:52:A:THR:HG23 | 1:36:A:THR:HG21 | 8        | 0.14          |
| (2,1158) | 1:52:A:THR:HG23 | 1:36:A:THR:HG22 | 8        | 0.14          |
| (2,1158) | 1:52:A:THR:HG23 | 1:36:A:THR:HG23 | 8        | 0.14          |
| (2,1058) | 1:33:A:ILE:HB   | 1:22:A:ASN:HD22 | 2        | 0.14          |
| (2,986)  | 1:11:A:GLU:HB3  | 1:11:A:GLU:HB2  | 6        | 0.14          |
| (2,948)  | 1:111:A:LEU:HB2 | 1:112:A:HIS:HA  | 6        | 0.14          |
| (2,948)  | 1:111:A:LEU:HB2 | 1:112:A:HIS:HA  | 9        | 0.14          |
| (2,848)  | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 1        | 0.14          |
| (2,848)  | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 8        | 0.14          |
| (2,582)  | 1:36:A:THR:HG21 | 1:51:A:LEU:H    | 2        | 0.14          |
| (2,582)  | 1:36:A:THR:HG22 | 1:51:A:LEU:H    | 2        | 0.14          |
| (2,582)  | 1:36:A:THR:HG23 | 1:51:A:LEU:H    | 2        | 0.14          |
| (2,528)  | 1:22:A:ASN:HA   | 1:33:A:ILE:HB   | 7        | 0.14          |
| (2,510)  | 1:19:A:ASP:HA   | 1:18:A:MET:HA   | 6        | 0.14          |
| (2,404)  | 1:56:A:ASN:HB2  | 1:56:A:ASN:HB3  | 2        | 0.14          |
| (2,404)  | 1:56:A:ASN:HB2  | 1:56:A:ASN:HB3  | 5        | 0.14          |
| (2,404)  | 1:56:A:ASN:HB2  | 1:56:A:ASN:HB3  | 8        | 0.14          |
| (2,404)  | 1:56:A:ASN:HB2  | 1:56:A:ASN:HB3  | 10       | 0.14          |
| (2,239)  | 1:50:A:PHE:HB3  | 1:95:A:ASP:HA   | 7        | 0.14          |
| (2,234)  | 1:49:A:VAL:HG21 | 1:35:A:ILE:HA   | 4        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,234)  | 1:49:A:VAL:HG22 | 1:35:A:ILE:HA   | 4        | 0.14          |
| (2,234)  | 1:49:A:VAL:HG23 | 1:35:A:ILE:HA   | 4        | 0.14          |
| (2,234)  | 1:49:A:VAL:HG21 | 1:35:A:ILE:HA   | 6        | 0.14          |
| (2,234)  | 1:49:A:VAL:HG22 | 1:35:A:ILE:HA   | 6        | 0.14          |
| (2,234)  | 1:49:A:VAL:HG23 | 1:35:A:ILE:HA   | 6        | 0.14          |
| (2,234)  | 1:49:A:VAL:HG21 | 1:35:A:ILE:HA   | 8        | 0.14          |
| (2,234)  | 1:49:A:VAL:HG22 | 1:35:A:ILE:HA   | 8        | 0.14          |
| (2,234)  | 1:49:A:VAL:HG23 | 1:35:A:ILE:HA   | 8        | 0.14          |
| (2,215)  | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB3  | 6        | 0.14          |
| (2,215)  | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB3  | 6        | 0.14          |
| (2,215)  | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB3  | 6        | 0.14          |
| (2,175)  | 1:72:A:GLY:HA3  | 1:75:A:LYS:HB3  | 1        | 0.14          |
| (2,175)  | 1:72:A:GLY:HA3  | 1:75:A:LYS:HB3  | 8        | 0.14          |
| (2,136)  | 1:31:A:GLY:HA2  | 1:54:A:LEU:HB3  | 1        | 0.14          |
| (2,120)  | 1:33:A:ILE:HA   | 1:53:A:VAL:HA   | 2        | 0.14          |
| (2,94)   | 1:60:A:VAL:C    | 1:64:A:PHE:N    | 1        | 0.14          |
| (2,94)   | 1:60:A:VAL:C    | 1:64:A:PHE:N    | 2        | 0.14          |
| (2,87)   | 1:63:A:THR:C    | 1:67:A:LEU:H    | 1        | 0.14          |
| (2,87)   | 1:63:A:THR:C    | 1:67:A:LEU:H    | 4        | 0.14          |
| (2,87)   | 1:63:A:THR:C    | 1:67:A:LEU:H    | 6        | 0.14          |
| (2,74)   | 1:73:A:PHE:C    | 1:77:A:GLU:N    | 10       | 0.14          |
| (2,32)   | 1:18:A:MET:C    | 1:22:A:ASN:N    | 3        | 0.14          |
| (2,31)   | 1:18:A:MET:C    | 1:22:A:ASN:H    | 4        | 0.14          |
| (2,31)   | 1:18:A:MET:C    | 1:22:A:ASN:H    | 5        | 0.14          |
| (2,31)   | 1:18:A:MET:C    | 1:22:A:ASN:H    | 9        | 0.14          |
| (2,14)   | 1:9:A:VAL:C     | 1:13:A:MET:N    | 7        | 0.14          |
| (1,153)  | 1:63:A:THR:O    | 1:67:A:LEU:H    | 8        | 0.14          |
| (1,137)  | 1:48:A:LYS:O    | 1:39:A:VAL:H    | 1        | 0.14          |
| (1,137)  | 1:48:A:LYS:O    | 1:39:A:VAL:H    | 2        | 0.14          |
| (1,137)  | 1:48:A:LYS:O    | 1:39:A:VAL:H    | 8        | 0.14          |
| (1,127)  | 1:20:A:ILE:O    | 1:24:A:LYS:H    | 6        | 0.14          |
| (1,119)  | 1:12:A:GLN:O    | 1:16:A:GLU:H    | 7        | 0.14          |
| (1,118)  | 1:11:A:GLU:O    | 1:15:A:LYS:H    | 7        | 0.14          |
| (1,117)  | 1:10:A:GLY:O    | 1:14:A:LYS:H    | 3        | 0.14          |
| (1,116)  | 1:9:A:VAL:O     | 1:13:A:MET:H    | 9        | 0.14          |
| (1,43)   | 1:68:A:ASP:H    | 1:64:A:PHE:O    | 7        | 0.14          |
| (1,42)   | 1:69:A:LYS:H    | 1:65:A:LYS:O    | 4        | 0.14          |
| (1,39)   | 1:75:A:LYS:H    | 1:71:A:LYS:O    | 9        | 0.14          |
| (2,2975) | 1:96:A:GLN:H    | 1:96:A:GLN:HE22 | 6        | 0.13          |
| (2,2960) | 1:91:A:MET:H    | 1:92:A:TYR:HA   | 3        | 0.13          |
| (2,2959) | 1:91:A:MET:H    | 1:47:A:ALA:HA   | 9        | 0.13          |
| (2,2912) | 1:76:A:SER:H    | 1:77:A:GLU:HB3  | 6        | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (2,2856) | 1:63:A:THR:H   | 1:65:A:LYS:HG2  | 1        | 0.13          |
| (2,2772) | 1:49:A:VAL:H   | 1:38:A:VAL:HG21 | 2        | 0.13          |
| (2,2772) | 1:49:A:VAL:H   | 1:38:A:VAL:HG22 | 2        | 0.13          |
| (2,2772) | 1:49:A:VAL:H   | 1:38:A:VAL:HG23 | 2        | 0.13          |
| (2,2772) | 1:49:A:VAL:H   | 1:38:A:VAL:HG21 | 4        | 0.13          |
| (2,2772) | 1:49:A:VAL:H   | 1:38:A:VAL:HG22 | 4        | 0.13          |
| (2,2772) | 1:49:A:VAL:H   | 1:38:A:VAL:HG23 | 4        | 0.13          |
| (2,2772) | 1:49:A:VAL:H   | 1:38:A:VAL:HG21 | 7        | 0.13          |
| (2,2772) | 1:49:A:VAL:H   | 1:38:A:VAL:HG22 | 7        | 0.13          |
| (2,2772) | 1:49:A:VAL:H   | 1:38:A:VAL:HG23 | 7        | 0.13          |
| (2,2743) | 1:45:A:SER:H   | 1:46:A:GLN:HA   | 4        | 0.13          |
| (2,2737) | 1:43:A:ASP:H   | 1:45:A:SER:HB3  | 2        | 0.13          |
| (2,2681) | 1:34:A:THR:H   | 1:51:A:LEU:HB2  | 8        | 0.13          |
| (2,2681) | 1:34:A:THR:H   | 1:51:A:LEU:HB2  | 10       | 0.13          |
| (2,2657) | 1:23:A:ASN:H   | 1:23:A:ASN:HD22 | 6        | 0.13          |
| (2,2464) | 1:66:A:ALA:H   | 1:65:A:LYS:HG2  | 3        | 0.13          |
| (2,2428) | 1:58:A:LYS:H   | 1:56:A:ASN:HA   | 8        | 0.13          |
| (2,2382) | 1:48:A:LYS:H   | 1:48:A:LYS:HD3  | 8        | 0.13          |
| (2,2096) | 1:102:A:ASN:H  | 1:101:A:GLY:HA2 | 1        | 0.13          |
| (2,2088) | 1:99:A:GLU:H   | 1:98:A:ILE:HG13 | 5        | 0.13          |
| (2,2054) | 1:89:A:GLU:H   | 1:46:A:GLN:HG2  | 5        | 0.13          |
| (2,1907) | 1:40:A:LEU:H   | 1:38:A:VAL:HG21 | 9        | 0.13          |
| (2,1907) | 1:40:A:LEU:H   | 1:38:A:VAL:HG22 | 9        | 0.13          |
| (2,1907) | 1:40:A:LEU:H   | 1:38:A:VAL:HG23 | 9        | 0.13          |
| (2,1900) | 1:38:A:VAL:H   | 1:39:A:VAL:HG21 | 1        | 0.13          |
| (2,1900) | 1:38:A:VAL:H   | 1:39:A:VAL:HG22 | 1        | 0.13          |
| (2,1900) | 1:38:A:VAL:H   | 1:39:A:VAL:HG23 | 1        | 0.13          |
| (2,1688) | 1:77:A:GLU:H   | 1:73:A:PHE:HA   | 8        | 0.13          |
| (2,1599) | 1:62:A:ASN:H   | 1:64:A:PHE:HB3  | 7        | 0.13          |
| (2,1575) | 1:58:A:LYS:H   | 1:59:A:GLU:HG3  | 5        | 0.13          |
| (2,1495) | 1:46:A:GLN:H   | 1:45:A:SER:H    | 2        | 0.13          |
| (2,995)  | 1:13:A:MET:HB3 | 1:10:A:GLY:HA3  | 9        | 0.13          |
| (2,995)  | 1:13:A:MET:HB3 | 1:10:A:GLY:HA3  | 10       | 0.13          |
| (2,994)  | 1:13:A:MET:HB3 | 1:38:A:VAL:HB   | 1        | 0.13          |
| (2,986)  | 1:11:A:GLU:HB3 | 1:11:A:GLU:HB2  | 1        | 0.13          |
| (2,986)  | 1:11:A:GLU:HB3 | 1:11:A:GLU:HB2  | 2        | 0.13          |
| (2,986)  | 1:11:A:GLU:HB3 | 1:11:A:GLU:HB2  | 3        | 0.13          |
| (2,986)  | 1:11:A:GLU:HB3 | 1:11:A:GLU:HB2  | 4        | 0.13          |
| (2,986)  | 1:11:A:GLU:HB3 | 1:11:A:GLU:HB2  | 5        | 0.13          |
| (2,986)  | 1:11:A:GLU:HB3 | 1:11:A:GLU:HB2  | 7        | 0.13          |
| (2,986)  | 1:11:A:GLU:HB3 | 1:11:A:GLU:HB2  | 8        | 0.13          |
| (2,986)  | 1:11:A:GLU:HB3 | 1:11:A:GLU:HB2  | 9        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,986) | 1:11:A:GLU:HB3  | 1:11:A:GLU:HB2  | 10       | 0.13          |
| (2,948) | 1:111:A:LEU:HB2 | 1:112:A:HIS:HA  | 8        | 0.13          |
| (2,941) | 1:111:A:LEU:HA  | 1:110:A:ASP:H   | 1        | 0.13          |
| (2,919) | 1:108:A:ILE:HA  | 1:110:A:ASP:HB2 | 6        | 0.13          |
| (2,883) | 1:81:A:ARG:HB3  | 1:80:A:SER:H    | 7        | 0.13          |
| (2,848) | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 9        | 0.13          |
| (2,760) | 1:62:A:ASN:HB2  | 1:59:A:GLU:HA   | 2        | 0.13          |
| (2,737) | 1:59:A:GLU:HG3  | 1:56:A:ASN:H    | 8        | 0.13          |
| (2,510) | 1:19:A:ASP:HA   | 1:18:A:MET:HA   | 4        | 0.13          |
| (2,510) | 1:19:A:ASP:HA   | 1:18:A:MET:HA   | 5        | 0.13          |
| (2,437) | 1:6:A:ALA:HB1   | 1:39:A:VAL:HG21 | 6        | 0.13          |
| (2,437) | 1:6:A:ALA:HB1   | 1:39:A:VAL:HG22 | 6        | 0.13          |
| (2,437) | 1:6:A:ALA:HB1   | 1:39:A:VAL:HG23 | 6        | 0.13          |
| (2,437) | 1:6:A:ALA:HB2   | 1:39:A:VAL:HG21 | 6        | 0.13          |
| (2,437) | 1:6:A:ALA:HB2   | 1:39:A:VAL:HG22 | 6        | 0.13          |
| (2,437) | 1:6:A:ALA:HB2   | 1:39:A:VAL:HG23 | 6        | 0.13          |
| (2,437) | 1:6:A:ALA:HB3   | 1:39:A:VAL:HG21 | 6        | 0.13          |
| (2,437) | 1:6:A:ALA:HB3   | 1:39:A:VAL:HG22 | 6        | 0.13          |
| (2,437) | 1:6:A:ALA:HB3   | 1:39:A:VAL:HG23 | 6        | 0.13          |
| (2,404) | 1:56:A:ASN:HB2  | 1:56:A:ASN:HB3  | 1        | 0.13          |
| (2,404) | 1:56:A:ASN:HB2  | 1:56:A:ASN:HB3  | 3        | 0.13          |
| (2,404) | 1:56:A:ASN:HB2  | 1:56:A:ASN:HB3  | 4        | 0.13          |
| (2,404) | 1:56:A:ASN:HB2  | 1:56:A:ASN:HB3  | 6        | 0.13          |
| (2,404) | 1:56:A:ASN:HB2  | 1:56:A:ASN:HB3  | 7        | 0.13          |
| (2,404) | 1:56:A:ASN:HB2  | 1:56:A:ASN:HB3  | 9        | 0.13          |
| (2,281) | 1:10:A:GLY:HA2  | 1:38:A:VAL:HB   | 4        | 0.13          |
| (2,261) | 1:94:A:TYR:HE1  | 1:53:A:VAL:H    | 8        | 0.13          |
| (2,261) | 1:94:A:TYR:HE2  | 1:53:A:VAL:H    | 8        | 0.13          |
| (2,215) | 1:17:A:LEU:HD21 | 1:78:A:LEU:HB3  | 4        | 0.13          |
| (2,215) | 1:17:A:LEU:HD22 | 1:78:A:LEU:HB3  | 4        | 0.13          |
| (2,215) | 1:17:A:LEU:HD23 | 1:78:A:LEU:HB3  | 4        | 0.13          |
| (2,208) | 1:79:A:GLY:HA2  | 1:76:A:SER:HA   | 3        | 0.13          |
| (2,175) | 1:72:A:GLY:HA3  | 1:75:A:LYS:HB3  | 9        | 0.13          |
| (2,155) | 1:66:A:ALA:HB1  | 1:25:A:VAL:HG21 | 5        | 0.13          |
| (2,155) | 1:66:A:ALA:HB1  | 1:25:A:VAL:HG22 | 5        | 0.13          |
| (2,155) | 1:66:A:ALA:HB1  | 1:25:A:VAL:HG23 | 5        | 0.13          |
| (2,155) | 1:66:A:ALA:HB2  | 1:25:A:VAL:HG21 | 5        | 0.13          |
| (2,155) | 1:66:A:ALA:HB2  | 1:25:A:VAL:HG22 | 5        | 0.13          |
| (2,155) | 1:66:A:ALA:HB2  | 1:25:A:VAL:HG23 | 5        | 0.13          |
| (2,155) | 1:66:A:ALA:HB3  | 1:25:A:VAL:HG21 | 5        | 0.13          |
| (2,155) | 1:66:A:ALA:HB3  | 1:25:A:VAL:HG22 | 5        | 0.13          |
| (2,155) | 1:66:A:ALA:HB3  | 1:25:A:VAL:HG23 | 5        | 0.13          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (2,93)   | 1:60:A:VAL:C  | 1:64:A:PHE:H    | 3        | 0.13          |
| (2,93)   | 1:60:A:VAL:C  | 1:64:A:PHE:H    | 8        | 0.13          |
| (2,87)   | 1:63:A:THR:C  | 1:67:A:LEU:H    | 5        | 0.13          |
| (2,31)   | 1:18:A:MET:C  | 1:22:A:ASN:H    | 2        | 0.13          |
| (2,29)   | 1:17:A:LEU:C  | 1:21:A:ILE:H    | 8        | 0.13          |
| (2,29)   | 1:17:A:LEU:C  | 1:21:A:ILE:H    | 10       | 0.13          |
| (2,25)   | 1:15:A:LYS:C  | 1:19:A:ASP:H    | 5        | 0.13          |
| (2,25)   | 1:15:A:LYS:C  | 1:19:A:ASP:H    | 10       | 0.13          |
| (2,20)   | 1:12:A:GLN:C  | 1:16:A:GLU:N    | 2        | 0.13          |
| (2,20)   | 1:12:A:GLN:C  | 1:16:A:GLU:N    | 8        | 0.13          |
| (2,17)   | 1:11:A:GLU:C  | 1:15:A:LYS:H    | 1        | 0.13          |
| (2,11)   | 1:8:A:ARG:C   | 1:12:A:GLN:H    | 1        | 0.13          |
| (2,11)   | 1:8:A:ARG:C   | 1:12:A:GLN:H    | 6        | 0.13          |
| (2,6)    | 1:5:A:ARG:C   | 1:9:A:VAL:N     | 9        | 0.13          |
| (2,5)    | 1:5:A:ARG:C   | 1:9:A:VAL:H     | 5        | 0.13          |
| (2,5)    | 1:5:A:ARG:C   | 1:9:A:VAL:H     | 9        | 0.13          |
| (1,159)  | 1:57:A:ASP:O  | 1:61:A:GLU:H    | 7        | 0.13          |
| (1,159)  | 1:57:A:ASP:O  | 1:61:A:GLU:H    | 10       | 0.13          |
| (1,153)  | 1:63:A:THR:O  | 1:67:A:LEU:H    | 6        | 0.13          |
| (1,127)  | 1:20:A:ILE:O  | 1:24:A:LYS:H    | 1        | 0.13          |
| (1,127)  | 1:20:A:ILE:O  | 1:24:A:LYS:H    | 7        | 0.13          |
| (1,118)  | 1:11:A:GLU:O  | 1:15:A:LYS:H    | 9        | 0.13          |
| (1,117)  | 1:10:A:GLY:O  | 1:14:A:LYS:H    | 1        | 0.13          |
| (1,116)  | 1:9:A:VAL:O   | 1:13:A:MET:H    | 1        | 0.13          |
| (1,46)   | 1:65:A:LYS:H  | 1:61:A:GLU:O    | 5        | 0.13          |
| (1,46)   | 1:65:A:LYS:H  | 1:61:A:GLU:O    | 8        | 0.13          |
| (1,46)   | 1:65:A:LYS:H  | 1:61:A:GLU:O    | 10       | 0.13          |
| (1,42)   | 1:69:A:LYS:H  | 1:65:A:LYS:O    | 2        | 0.13          |
| (2,3023) | 1:112:A:HIS:H | 1:113:A:LYS:H   | 3        | 0.12          |
| (2,2991) | 1:98:A:ILE:H  | 1:99:A:GLU:HA   | 9        | 0.12          |
| (2,2975) | 1:96:A:GLN:H  | 1:96:A:GLN:HE22 | 9        | 0.12          |
| (2,2959) | 1:91:A:MET:H  | 1:47:A:ALA:HA   | 1        | 0.12          |
| (2,2913) | 1:77:A:GLU:H  | 1:78:A:LEU:HB2  | 5        | 0.12          |
| (2,2913) | 1:77:A:GLU:H  | 1:78:A:LEU:HB2  | 9        | 0.12          |
| (2,2758) | 1:47:A:ALA:H  | 1:89:A:GLU:HB3  | 4        | 0.12          |
| (2,2758) | 1:47:A:ALA:H  | 1:89:A:GLU:HB3  | 7        | 0.12          |
| (2,2743) | 1:45:A:SER:H  | 1:46:A:GLN:HA   | 10       | 0.12          |
| (2,2692) | 1:35:A:ILE:H  | 1:36:A:THR:HA   | 3        | 0.12          |
| (2,2692) | 1:35:A:ILE:H  | 1:36:A:THR:HA   | 4        | 0.12          |
| (2,2692) | 1:35:A:ILE:H  | 1:36:A:THR:HA   | 6        | 0.12          |
| (2,2657) | 1:23:A:ASN:H  | 1:23:A:ASN:HD22 | 7        | 0.12          |
| (2,2657) | 1:23:A:ASN:H  | 1:23:A:ASN:HD22 | 8        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2588) | 1:22:A:ASN:H    | 1:22:A:ASN:HD22 | 1        | 0.12          |
| (2,2588) | 1:22:A:ASN:H    | 1:22:A:ASN:HD22 | 2        | 0.12          |
| (2,2588) | 1:22:A:ASN:H    | 1:22:A:ASN:HD22 | 6        | 0.12          |
| (2,2588) | 1:22:A:ASN:H    | 1:22:A:ASN:HD22 | 9        | 0.12          |
| (2,2428) | 1:58:A:LYS:H    | 1:56:A:ASN:HA   | 6        | 0.12          |
| (2,2088) | 1:99:A:GLU:H    | 1:98:A:ILE:HG13 | 1        | 0.12          |
| (2,2054) | 1:89:A:GLU:H    | 1:46:A:GLN:HG2  | 6        | 0.12          |
| (2,2025) | 1:73:A:PHE:H    | 1:71:A:LYS:HB2  | 6        | 0.12          |
| (2,1876) | 1:34:A:THR:H    | 1:52:A:THR:HB   | 10       | 0.12          |
| (2,1701) | 1:79:A:GLY:H    | 1:75:A:LYS:HB3  | 5        | 0.12          |
| (2,1617) | 1:66:A:ALA:H    | 1:69:A:LYS:HB3  | 1        | 0.12          |
| (2,1617) | 1:66:A:ALA:H    | 1:69:A:LYS:HB3  | 7        | 0.12          |
| (2,1599) | 1:62:A:ASN:H    | 1:64:A:PHE:HB3  | 4        | 0.12          |
| (2,1575) | 1:58:A:LYS:H    | 1:59:A:GLU:HG3  | 3        | 0.12          |
| (2,1575) | 1:58:A:LYS:H    | 1:59:A:GLU:HG3  | 6        | 0.12          |
| (2,1389) | 1:15:A:LYS:H    | 1:16:A:GLU:HB2  | 10       | 0.12          |
| (2,1344) | 1:98:A:ILE:HG12 | 1:95:A:ASP:HB2  | 3        | 0.12          |
| (2,1296) | 1:76:A:SER:HB3  | 1:73:A:PHE:HA   | 4        | 0.12          |
| (2,1280) | 1:74:A:ILE:HA   | 1:25:A:VAL:HG11 | 10       | 0.12          |
| (2,1280) | 1:74:A:ILE:HA   | 1:25:A:VAL:HG12 | 10       | 0.12          |
| (2,1280) | 1:74:A:ILE:HA   | 1:25:A:VAL:HG13 | 10       | 0.12          |
| (2,1247) | 1:68:A:ASP:HB2  | 1:71:A:LYS:HG3  | 9        | 0.12          |
| (2,1227) | 1:65:A:LYS:HG2  | 1:61:A:GLU:HB2  | 6        | 0.12          |
| (2,1199) | 1:59:A:GLU:HB2  | 1:56:A:ASN:HD22 | 9        | 0.12          |
| (2,1155) | 1:52:A:THR:HB   | 1:34:A:THR:HG1  | 4        | 0.12          |
| (2,1155) | 1:52:A:THR:HB   | 1:34:A:THR:HG1  | 9        | 0.12          |
| (2,1139) | 1:50:A:PHE:HA   | 1:50:A:PHE:HD1  | 10       | 0.12          |
| (2,1139) | 1:50:A:PHE:HA   | 1:50:A:PHE:HD2  | 10       | 0.12          |
| (2,785)  | 1:65:A:LYS:HD2  | 1:65:A:LYS:HA   | 1        | 0.12          |
| (2,785)  | 1:65:A:LYS:HD2  | 1:65:A:LYS:HA   | 2        | 0.12          |
| (2,760)  | 1:62:A:ASN:HB2  | 1:59:A:GLU:HA   | 9        | 0.12          |
| (2,528)  | 1:22:A:ASN:HA   | 1:33:A:ILE:HB   | 2        | 0.12          |
| (2,419)  | 1:73:A:PHE:HB3  | 1:73:A:PHE:HB2  | 1        | 0.12          |
| (2,419)  | 1:73:A:PHE:HB3  | 1:73:A:PHE:HB2  | 2        | 0.12          |
| (2,419)  | 1:73:A:PHE:HB3  | 1:73:A:PHE:HB2  | 3        | 0.12          |
| (2,419)  | 1:73:A:PHE:HB3  | 1:73:A:PHE:HB2  | 4        | 0.12          |
| (2,419)  | 1:73:A:PHE:HB3  | 1:73:A:PHE:HB2  | 5        | 0.12          |
| (2,419)  | 1:73:A:PHE:HB3  | 1:73:A:PHE:HB2  | 6        | 0.12          |
| (2,419)  | 1:73:A:PHE:HB3  | 1:73:A:PHE:HB2  | 7        | 0.12          |
| (2,419)  | 1:73:A:PHE:HB3  | 1:73:A:PHE:HB2  | 8        | 0.12          |
| (2,419)  | 1:73:A:PHE:HB3  | 1:73:A:PHE:HB2  | 9        | 0.12          |
| (2,419)  | 1:73:A:PHE:HB3  | 1:73:A:PHE:HB2  | 10       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,415) | 1:73:A:PHE:HB2  | 1:73:A:PHE:HB3  | 1        | 0.12          |
| (2,415) | 1:73:A:PHE:HB2  | 1:73:A:PHE:HB3  | 2        | 0.12          |
| (2,415) | 1:73:A:PHE:HB2  | 1:73:A:PHE:HB3  | 3        | 0.12          |
| (2,415) | 1:73:A:PHE:HB2  | 1:73:A:PHE:HB3  | 4        | 0.12          |
| (2,415) | 1:73:A:PHE:HB2  | 1:73:A:PHE:HB3  | 5        | 0.12          |
| (2,415) | 1:73:A:PHE:HB2  | 1:73:A:PHE:HB3  | 6        | 0.12          |
| (2,415) | 1:73:A:PHE:HB2  | 1:73:A:PHE:HB3  | 7        | 0.12          |
| (2,415) | 1:73:A:PHE:HB2  | 1:73:A:PHE:HB3  | 8        | 0.12          |
| (2,415) | 1:73:A:PHE:HB2  | 1:73:A:PHE:HB3  | 9        | 0.12          |
| (2,415) | 1:73:A:PHE:HB2  | 1:73:A:PHE:HB3  | 10       | 0.12          |
| (2,281) | 1:10:A:GLY:HA2  | 1:38:A:VAL:HB   | 1        | 0.12          |
| (2,281) | 1:10:A:GLY:HA2  | 1:38:A:VAL:HB   | 7        | 0.12          |
| (2,261) | 1:94:A:TYR:HE1  | 1:53:A:VAL:H    | 2        | 0.12          |
| (2,261) | 1:94:A:TYR:HE2  | 1:53:A:VAL:H    | 2        | 0.12          |
| (2,192) | 1:25:A:VAL:HG21 | 1:74:A:ILE:HA   | 4        | 0.12          |
| (2,192) | 1:25:A:VAL:HG22 | 1:74:A:ILE:HA   | 4        | 0.12          |
| (2,192) | 1:25:A:VAL:HG23 | 1:74:A:ILE:HA   | 4        | 0.12          |
| (2,191) | 1:74:A:ILE:HA   | 1:25:A:VAL:HG21 | 3        | 0.12          |
| (2,191) | 1:74:A:ILE:HA   | 1:25:A:VAL:HG22 | 3        | 0.12          |
| (2,191) | 1:74:A:ILE:HA   | 1:25:A:VAL:HG23 | 3        | 0.12          |
| (2,190) | 1:74:A:ILE:HA   | 1:25:A:VAL:HG11 | 10       | 0.12          |
| (2,190) | 1:74:A:ILE:HA   | 1:25:A:VAL:HG12 | 10       | 0.12          |
| (2,190) | 1:74:A:ILE:HA   | 1:25:A:VAL:HG13 | 10       | 0.12          |
| (2,160) | 1:67:A:LEU:HB2  | 1:64:A:PHE:HA   | 4        | 0.12          |
| (2,159) | 1:67:A:LEU:HA   | 1:25:A:VAL:HG21 | 4        | 0.12          |
| (2,159) | 1:67:A:LEU:HA   | 1:25:A:VAL:HG22 | 4        | 0.12          |
| (2,159) | 1:67:A:LEU:HA   | 1:25:A:VAL:HG23 | 4        | 0.12          |
| (2,136) | 1:31:A:GLY:HA2  | 1:54:A:LEU:HB3  | 3        | 0.12          |
| (2,121) | 1:45:A:SER:HA   | 1:88:A:PRO:HA   | 4        | 0.12          |
| (2,120) | 1:33:A:ILE:HA   | 1:53:A:VAL:HA   | 4        | 0.12          |
| (2,110) | 1:89:A:GLU:C    | 1:47:A:ALA:N    | 10       | 0.12          |
| (2,95)  | 1:59:A:GLU:C    | 1:63:A:THR:H    | 10       | 0.12          |
| (2,94)  | 1:60:A:VAL:C    | 1:64:A:PHE:N    | 8        | 0.12          |
| (2,93)  | 1:60:A:VAL:C    | 1:64:A:PHE:H    | 4        | 0.12          |
| (2,93)  | 1:60:A:VAL:C    | 1:64:A:PHE:H    | 5        | 0.12          |
| (2,81)  | 1:66:A:ALA:C    | 1:70:A:ALA:H    | 2        | 0.12          |
| (2,70)  | 1:75:A:LYS:C    | 1:79:A:GLY:N    | 10       | 0.12          |
| (2,67)  | 1:76:A:SER:C    | 1:80:A:SER:H    | 7        | 0.12          |
| (2,64)  | 1:89:A:GLU:C    | 1:47:A:ALA:N    | 10       | 0.12          |
| (2,26)  | 1:15:A:LYS:C    | 1:19:A:ASP:N    | 9        | 0.12          |
| (2,25)  | 1:15:A:LYS:C    | 1:19:A:ASP:H    | 6        | 0.12          |
| (2,19)  | 1:12:A:GLN:C    | 1:16:A:GLU:H    | 6        | 0.12          |

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| Key      | Atom-1       | Atom-2          | Model ID | Violation (Å) |
|----------|--------------|-----------------|----------|---------------|
| (2,19)   | 1:12:A:GLN:C | 1:16:A:GLU:H    | 9        | 0.12          |
| (2,17)   | 1:11:A:GLU:C | 1:15:A:LYS:H    | 9        | 0.12          |
| (2,13)   | 1:9:A:VAL:C  | 1:13:A:MET:H    | 9        | 0.12          |
| (2,11)   | 1:8:A:ARG:C  | 1:12:A:GLN:H    | 2        | 0.12          |
| (2,11)   | 1:8:A:ARG:C  | 1:12:A:GLN:H    | 9        | 0.12          |
| (2,6)    | 1:5:A:ARG:C  | 1:9:A:VAL:N     | 5        | 0.12          |
| (1,156)  | 1:60:A:VAL:O | 1:64:A:PHE:H    | 3        | 0.12          |
| (1,153)  | 1:63:A:THR:O | 1:67:A:LEU:H    | 9        | 0.12          |
| (1,153)  | 1:63:A:THR:O | 1:67:A:LEU:H    | 10       | 0.12          |
| (1,150)  | 1:66:A:ALA:O | 1:70:A:ALA:H    | 2        | 0.12          |
| (1,139)  | 1:39:A:VAL:O | 1:48:A:LYS:H    | 5        | 0.12          |
| (1,137)  | 1:48:A:LYS:O | 1:39:A:VAL:H    | 7        | 0.12          |
| (1,122)  | 1:15:A:LYS:O | 1:19:A:ASP:H    | 1        | 0.12          |
| (1,122)  | 1:15:A:LYS:O | 1:19:A:ASP:H    | 9        | 0.12          |
| (1,119)  | 1:12:A:GLN:O | 1:16:A:GLU:H    | 1        | 0.12          |
| (1,116)  | 1:9:A:VAL:O  | 1:13:A:MET:H    | 4        | 0.12          |
| (1,115)  | 1:8:A:ARG:O  | 1:12:A:GLN:H    | 7        | 0.12          |
| (1,42)   | 1:69:A:LYS:H | 1:65:A:LYS:O    | 8        | 0.12          |
| (2,2959) | 1:91:A:MET:H | 1:47:A:ALA:HA   | 7        | 0.11          |
| (2,2959) | 1:91:A:MET:H | 1:47:A:ALA:HA   | 10       | 0.11          |
| (2,2913) | 1:77:A:GLU:H | 1:78:A:LEU:HB2  | 3        | 0.11          |
| (2,2912) | 1:76:A:SER:H | 1:77:A:GLU:HB3  | 1        | 0.11          |
| (2,2886) | 1:71:A:LYS:H | 1:69:A:LYS:HB3  | 10       | 0.11          |
| (2,2856) | 1:63:A:THR:H | 1:65:A:LYS:HG2  | 6        | 0.11          |
| (2,2856) | 1:63:A:THR:H | 1:65:A:LYS:HG2  | 9        | 0.11          |
| (2,2819) | 1:58:A:LYS:H | 1:59:A:GLU:HB2  | 8        | 0.11          |
| (2,2758) | 1:47:A:ALA:H | 1:89:A:GLU:HB3  | 9        | 0.11          |
| (2,2743) | 1:45:A:SER:H | 1:46:A:GLN:HA   | 8        | 0.11          |
| (2,2738) | 1:43:A:ASP:H | 1:41:A:THR:HG1  | 5        | 0.11          |
| (2,2738) | 1:43:A:ASP:H | 1:41:A:THR:HG1  | 7        | 0.11          |
| (2,2464) | 1:66:A:ALA:H | 1:65:A:LYS:HG2  | 1        | 0.11          |
| (2,2398) | 1:49:A:VAL:H | 1:50:A:PHE:HD1  | 7        | 0.11          |
| (2,2398) | 1:49:A:VAL:H | 1:50:A:PHE:HD2  | 7        | 0.11          |
| (2,2398) | 1:49:A:VAL:H | 1:50:A:PHE:HD1  | 10       | 0.11          |
| (2,2398) | 1:49:A:VAL:H | 1:50:A:PHE:HD2  | 10       | 0.11          |
| (2,2338) | 1:35:A:ILE:H | 1:36:A:THR:HG21 | 1        | 0.11          |
| (2,2338) | 1:35:A:ILE:H | 1:36:A:THR:HG22 | 1        | 0.11          |
| (2,2338) | 1:35:A:ILE:H | 1:36:A:THR:HG23 | 1        | 0.11          |
| (2,2338) | 1:35:A:ILE:H | 1:36:A:THR:HG21 | 10       | 0.11          |
| (2,2338) | 1:35:A:ILE:H | 1:36:A:THR:HG22 | 10       | 0.11          |
| (2,2338) | 1:35:A:ILE:H | 1:36:A:THR:HG23 | 10       | 0.11          |
| (2,2268) | 1:17:A:LEU:H | 1:15:A:LYS:HB2  | 8        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2118) | 1:112:A:HIS:H   | 1:78:A:LEU:HB3  | 10       | 0.11          |
| (2,2090) | 1:99:A:GLU:H    | 1:101:A:GLY:HA2 | 10       | 0.11          |
| (2,2062) | 1:91:A:MET:H    | 1:49:A:VAL:HB   | 8        | 0.11          |
| (2,2025) | 1:73:A:PHE:H    | 1:71:A:LYS:HB2  | 7        | 0.11          |
| (2,2025) | 1:73:A:PHE:H    | 1:71:A:LYS:HB2  | 10       | 0.11          |
| (2,1992) | 1:64:A:PHE:H    | 1:62:A:ASN:HB2  | 4        | 0.11          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG21 | 3        | 0.11          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG22 | 3        | 0.11          |
| (2,1917) | 1:41:A:THR:H    | 1:39:A:VAL:HG23 | 3        | 0.11          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG21 | 1        | 0.11          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG22 | 1        | 0.11          |
| (2,1907) | 1:40:A:LEU:H    | 1:38:A:VAL:HG23 | 1        | 0.11          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG21 | 2        | 0.11          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG22 | 2        | 0.11          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG23 | 2        | 0.11          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG21 | 9        | 0.11          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG22 | 9        | 0.11          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG23 | 9        | 0.11          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG21 | 10       | 0.11          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG22 | 10       | 0.11          |
| (2,1900) | 1:38:A:VAL:H    | 1:39:A:VAL:HG23 | 10       | 0.11          |
| (2,1823) | 1:15:A:LYS:H    | 1:18:A:MET:HB2  | 6        | 0.11          |
| (2,1688) | 1:77:A:GLU:H    | 1:73:A:PHE:HA   | 1        | 0.11          |
| (2,1628) | 1:68:A:ASP:H    | 1:69:A:LYS:HB3  | 2        | 0.11          |
| (2,1575) | 1:58:A:LYS:H    | 1:59:A:GLU:HG3  | 8        | 0.11          |
| (2,1495) | 1:46:A:GLN:H    | 1:45:A:SER:H    | 8        | 0.11          |
| (2,1389) | 1:15:A:LYS:H    | 1:16:A:GLU:HB2  | 5        | 0.11          |
| (2,1344) | 1:98:A:ILE:HG12 | 1:95:A:ASP:HB2  | 6        | 0.11          |
| (2,1330) | 1:96:A:GLN:HG2  | 1:94:A:TYR:HD1  | 1        | 0.11          |
| (2,1330) | 1:96:A:GLN:HG2  | 1:94:A:TYR:HD2  | 1        | 0.11          |
| (2,1247) | 1:68:A:ASP:HB2  | 1:71:A:LYS:HG3  | 8        | 0.11          |
| (2,1227) | 1:65:A:LYS:HG2  | 1:61:A:GLU:HB2  | 2        | 0.11          |
| (2,1199) | 1:59:A:GLU:HB2  | 1:56:A:ASN:HD22 | 2        | 0.11          |
| (2,1199) | 1:59:A:GLU:HB2  | 1:56:A:ASN:HD22 | 7        | 0.11          |
| (2,1170) | 1:53:A:VAL:HB   | 1:51:A:LEU:HB2  | 8        | 0.11          |
| (2,1170) | 1:53:A:VAL:HB   | 1:51:A:LEU:HB2  | 10       | 0.11          |
| (2,1155) | 1:52:A:THR:HB   | 1:34:A:THR:HG1  | 1        | 0.11          |
| (2,1106) | 1:39:A:VAL:HG21 | 1:48:A:LYS:HB3  | 6        | 0.11          |
| (2,1106) | 1:39:A:VAL:HG22 | 1:48:A:LYS:HB3  | 6        | 0.11          |
| (2,1106) | 1:39:A:VAL:HG23 | 1:48:A:LYS:HB3  | 6        | 0.11          |
| (2,1093) | 1:38:A:VAL:HG21 | 1:10:A:GLY:HA3  | 10       | 0.11          |
| (2,1093) | 1:38:A:VAL:HG22 | 1:10:A:GLY:HA3  | 10       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1093) | 1:38:A:VAL:HG23 | 1:10:A:GLY:HA3  | 10       | 0.11          |
| (2,1092) | 1:38:A:VAL:HG21 | 1:17:A:LEU:HB3  | 5        | 0.11          |
| (2,1092) | 1:38:A:VAL:HG22 | 1:17:A:LEU:HB3  | 5        | 0.11          |
| (2,1092) | 1:38:A:VAL:HG23 | 1:17:A:LEU:HB3  | 5        | 0.11          |
| (2,917)  | 1:108:A:ILE:HA  | 1:107:A:MET:HB2 | 7        | 0.11          |
| (2,912)  | 1:107:A:MET:HA  | 1:108:A:ILE:HB  | 9        | 0.11          |
| (2,883)  | 1:81:A:ARG:HB3  | 1:80:A:SER:H    | 2        | 0.11          |
| (2,507)  | 1:19:A:ASP:HA   | 1:22:A:ASN:HB3  | 7        | 0.11          |
| (2,493)  | 1:16:A:GLU:HB2  | 1:17:A:LEU:HA   | 4        | 0.11          |
| (2,342)  | 1:38:A:VAL:HG21 | 1:10:A:GLY:HA2  | 8        | 0.11          |
| (2,342)  | 1:38:A:VAL:HG22 | 1:10:A:GLY:HA2  | 8        | 0.11          |
| (2,342)  | 1:38:A:VAL:HG23 | 1:10:A:GLY:HA2  | 8        | 0.11          |
| (2,281)  | 1:10:A:GLY:HA2  | 1:38:A:VAL:HB   | 9        | 0.11          |
| (2,254)  | 1:22:A:ASN:HD22 | 1:33:A:ILE:HB   | 3        | 0.11          |
| (2,210)  | 1:78:A:LEU:HA   | 1:16:A:GLU:HB2  | 1        | 0.11          |
| (2,192)  | 1:25:A:VAL:HG21 | 1:74:A:ILE:HA   | 1        | 0.11          |
| (2,192)  | 1:25:A:VAL:HG22 | 1:74:A:ILE:HA   | 1        | 0.11          |
| (2,192)  | 1:25:A:VAL:HG23 | 1:74:A:ILE:HA   | 1        | 0.11          |
| (2,136)  | 1:31:A:GLY:HA2  | 1:54:A:LEU:HB3  | 2        | 0.11          |
| (2,126)  | 1:93:A:GLU:H    | 1:50:A:PHE:HA   | 1        | 0.11          |
| (2,118)  | 1:38:A:VAL:HA   | 1:49:A:VAL:HA   | 8        | 0.11          |
| (2,94)   | 1:60:A:VAL:C    | 1:64:A:PHE:N    | 3        | 0.11          |
| (2,94)   | 1:60:A:VAL:C    | 1:64:A:PHE:N    | 4        | 0.11          |
| (2,94)   | 1:60:A:VAL:C    | 1:64:A:PHE:N    | 5        | 0.11          |
| (2,67)   | 1:76:A:SER:C    | 1:80:A:SER:H    | 3        | 0.11          |
| (2,55)   | 1:48:A:LYS:C    | 1:39:A:VAL:H    | 8        | 0.11          |
| (2,32)   | 1:18:A:MET:C    | 1:22:A:ASN:N    | 2        | 0.11          |
| (2,30)   | 1:17:A:LEU:C    | 1:21:A:ILE:N    | 10       | 0.11          |
| (2,29)   | 1:17:A:LEU:C    | 1:21:A:ILE:H    | 4        | 0.11          |
| (2,26)   | 1:15:A:LYS:C    | 1:19:A:ASP:N    | 10       | 0.11          |
| (2,20)   | 1:12:A:GLN:C    | 1:16:A:GLU:N    | 6        | 0.11          |
| (2,20)   | 1:12:A:GLN:C    | 1:16:A:GLU:N    | 9        | 0.11          |
| (2,13)   | 1:9:A:VAL:C     | 1:13:A:MET:H    | 6        | 0.11          |
| (2,12)   | 1:8:A:ARG:C     | 1:12:A:GLN:N    | 10       | 0.11          |
| (1,159)  | 1:57:A:ASP:O    | 1:61:A:GLU:H    | 1        | 0.11          |
| (1,159)  | 1:57:A:ASP:O    | 1:61:A:GLU:H    | 6        | 0.11          |
| (1,156)  | 1:60:A:VAL:O    | 1:64:A:PHE:H    | 1        | 0.11          |
| (1,118)  | 1:11:A:GLU:O    | 1:15:A:LYS:H    | 5        | 0.11          |
| (1,117)  | 1:10:A:GLY:O    | 1:14:A:LYS:H    | 4        | 0.11          |
| (1,117)  | 1:10:A:GLY:O    | 1:14:A:LYS:H    | 7        | 0.11          |
| (1,114)  | 1:7:A:GLU:O     | 1:11:A:GLU:H    | 10       | 0.11          |
| (1,51)   | 1:60:A:VAL:H    | 1:56:A:ASN:O    | 1        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,51)   | 1:60:A:VAL:H    | 1:56:A:ASN:O    | 7        | 0.11          |
| (1,39)   | 1:75:A:LYS:H    | 1:71:A:LYS:O    | 7        | 0.11          |
| (2,2991) | 1:98:A:ILE:H    | 1:99:A:GLU:HA   | 4        | 0.1           |
| (2,2856) | 1:63:A:THR:H    | 1:65:A:LYS:HG2  | 5        | 0.1           |
| (2,2750) | 1:46:A:GLN:H    | 1:46:A:GLN:HE22 | 2        | 0.1           |
| (2,2743) | 1:45:A:SER:H    | 1:46:A:GLN:HA   | 3        | 0.1           |
| (2,2739) | 1:44:A:LEU:H    | 1:41:A:THR:HG1  | 9        | 0.1           |
| (2,2556) | 1:89:A:GLU:H    | 1:46:A:GLN:HG3  | 1        | 0.1           |
| (2,2382) | 1:48:A:LYS:H    | 1:48:A:LYS:HD3  | 7        | 0.1           |
| (2,2096) | 1:102:A:ASN:H   | 1:101:A:GLY:HA2 | 2        | 0.1           |
| (2,2014) | 1:68:A:ASP:H    | 1:65:A:LYS:HB2  | 3        | 0.1           |
| (2,1787) | 1:29:A:ARG:HH11 | 1:29:A:ARG:HE   | 3        | 0.1           |
| (2,1715) | 1:89:A:GLU:H    | 1:46:A:GLN:HG3  | 1        | 0.1           |
| (2,1701) | 1:79:A:GLY:H    | 1:75:A:LYS:HB3  | 8        | 0.1           |
| (2,1616) | 1:66:A:ALA:H    | 1:65:A:LYS:HD2  | 6        | 0.1           |
| (2,1316) | 1:91:A:MET:HB2  | 1:48:A:LYS:HG3  | 4        | 0.1           |
| (2,1313) | 1:81:A:ARG:HB3  | 1:16:A:GLU:HB2  | 9        | 0.1           |
| (2,1002) | 1:16:A:GLU:HB2  | 1:81:A:ARG:HB3  | 9        | 0.1           |
| (2,995)  | 1:13:A:MET:HB3  | 1:10:A:GLY:HA3  | 6        | 0.1           |
| (2,960)  | 1:118:A:GLU:HA  | 1:117:A:VAL:HB  | 5        | 0.1           |
| (2,938)  | 1:111:A:LEU:HA  | 1:113:A:LYS:HB3 | 7        | 0.1           |
| (2,848)  | 1:75:A:LYS:HB3  | 1:72:A:GLY:HA3  | 4        | 0.1           |
| (2,737)  | 1:59:A:GLU:HG3  | 1:56:A:ASN:H    | 5        | 0.1           |
| (2,620)  | 1:40:A:LEU:HA   | 1:41:A:THR:H    | 10       | 0.1           |
| (2,510)  | 1:19:A:ASP:HA   | 1:18:A:MET:HA   | 1        | 0.1           |
| (2,254)  | 1:22:A:ASN:HD22 | 1:33:A:ILE:HB   | 1        | 0.1           |
| (2,210)  | 1:78:A:LEU:HA   | 1:16:A:GLU:HB2  | 4        | 0.1           |
| (2,175)  | 1:72:A:GLY:HA3  | 1:75:A:LYS:HB3  | 4        | 0.1           |
| (2,121)  | 1:45:A:SER:HA   | 1:88:A:PRO:HA   | 10       | 0.1           |
| (2,88)   | 1:63:A:THR:C    | 1:67:A:LEU:N    | 8        | 0.1           |
| (2,88)   | 1:63:A:THR:C    | 1:67:A:LEU:N    | 9        | 0.1           |
| (2,79)   | 1:70:A:ALA:C    | 1:74:A:ILE:H    | 5        | 0.1           |
| (2,79)   | 1:70:A:ALA:C    | 1:74:A:ILE:H    | 10       | 0.1           |
| (2,70)   | 1:75:A:LYS:C    | 1:79:A:GLY:N    | 7        | 0.1           |
| (2,31)   | 1:18:A:MET:C    | 1:22:A:ASN:H    | 8        | 0.1           |
| (2,26)   | 1:15:A:LYS:C    | 1:19:A:ASP:N    | 5        | 0.1           |
| (2,26)   | 1:15:A:LYS:C    | 1:19:A:ASP:N    | 6        | 0.1           |
| (2,25)   | 1:15:A:LYS:C    | 1:19:A:ASP:H    | 8        | 0.1           |
| (1,150)  | 1:66:A:ALA:O    | 1:70:A:ALA:H    | 1        | 0.1           |
| (1,143)  | 1:76:A:SER:O    | 1:80:A:SER:H    | 1        | 0.1           |
| (1,143)  | 1:76:A:SER:O    | 1:80:A:SER:H    | 2        | 0.1           |
| (1,139)  | 1:39:A:VAL:O    | 1:48:A:LYS:H    | 8        | 0.1           |

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| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (1,127) | 1:20:A:ILE:O | 1:24:A:LYS:H | 8        | 0.1           |
| (1,119) | 1:12:A:GLN:O | 1:16:A:GLU:H | 5        | 0.1           |
| (1,118) | 1:11:A:GLU:O | 1:15:A:LYS:H | 6        | 0.1           |
| (1,46)  | 1:65:A:LYS:H | 1:61:A:GLU:O | 4        | 0.1           |
| (1,46)  | 1:65:A:LYS:H | 1:61:A:GLU:O | 7        | 0.1           |
| (1,42)  | 1:69:A:LYS:H | 1:65:A:LYS:O | 10       | 0.1           |
| (1,39)  | 1:75:A:LYS:H | 1:71:A:LYS:O | 6        | 0.1           |

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

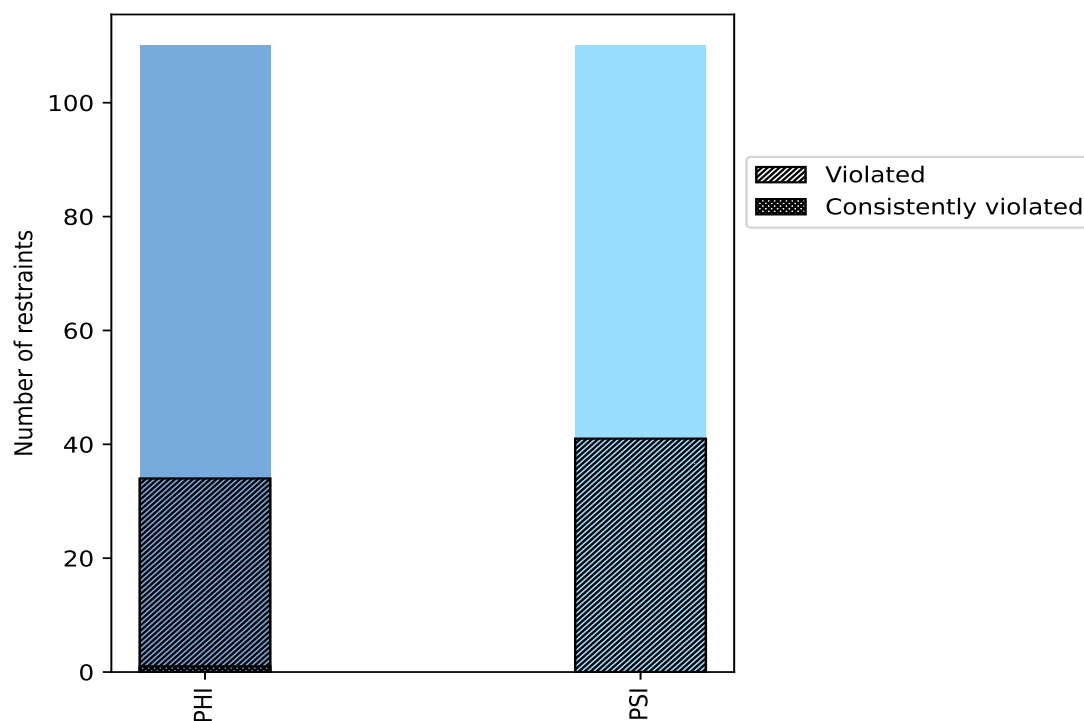
### 10.1 Summary of dihedral-angle violations [i](#)

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        | 110   | 50.0           | 34                    | 30.9           | 15.5           | 1                                  | 0.9            | 0.5            |
| PSI        | 110   | 50.0           | 41                    | 37.3           | 18.6           | 0                                  | 0.0            | 0.0            |
| Total      | 220   | 100.0          | 75                    | 34.1           | 34.1           | 1                                  | 0.5            | 0.5            |

<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](#)



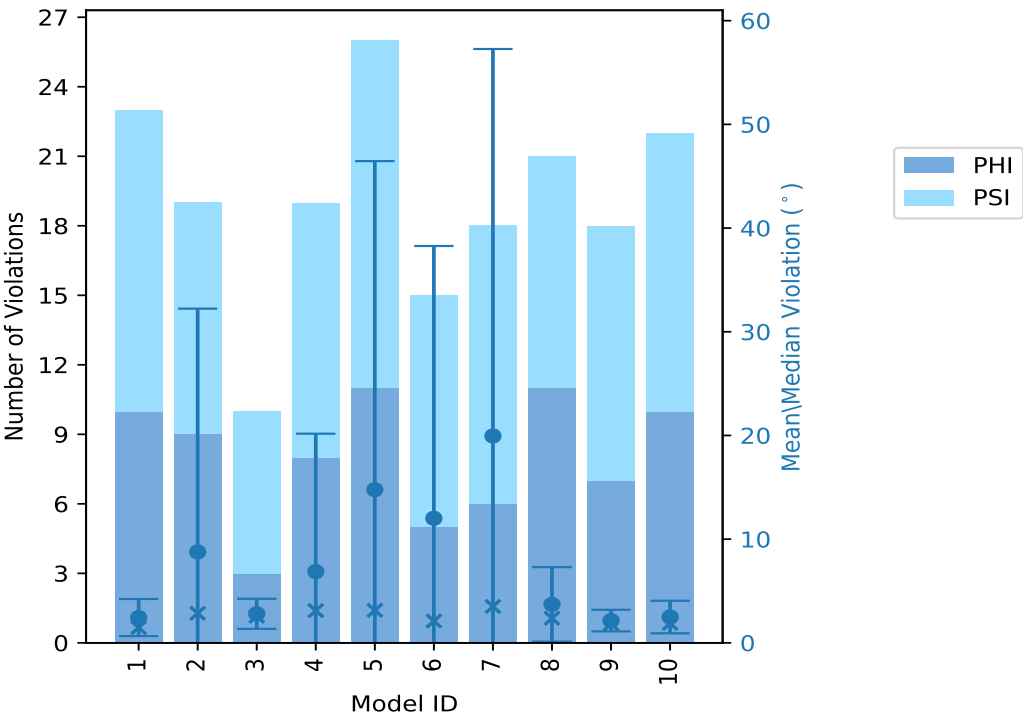
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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        | 10                   | 13  | 23    | 2.44     | 7.66    | 1.79   | 1.47       |
| 2        | 9                    | 10  | 19    | 8.77     | 107.91  | 23.46  | 2.85       |
| 3        | 3                    | 7   | 10    | 2.8      | 5.56    | 1.45   | 2.57       |
| 4        | 8                    | 11  | 19    | 6.87     | 59.65   | 13.3   | 3.11       |
| 5        | 11                   | 15  | 26    | 14.77    | 105.64  | 31.69  | 3.14       |
| 6        | 5                    | 10  | 15    | 12.01    | 107.71  | 26.26  | 2.11       |
| 7        | 6                    | 12  | 18    | 19.95    | 122.43  | 37.32  | 3.51       |
| 8        | 11                   | 10  | 21    | 3.71     | 14.27   | 3.59   | 2.37       |
| 9        | 7                    | 11  | 18    | 2.15     | 5.15    | 1.04   | 1.83       |
| 10       | 10                   | 12  | 22    | 2.49     | 7.38    | 1.57   | 1.88       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

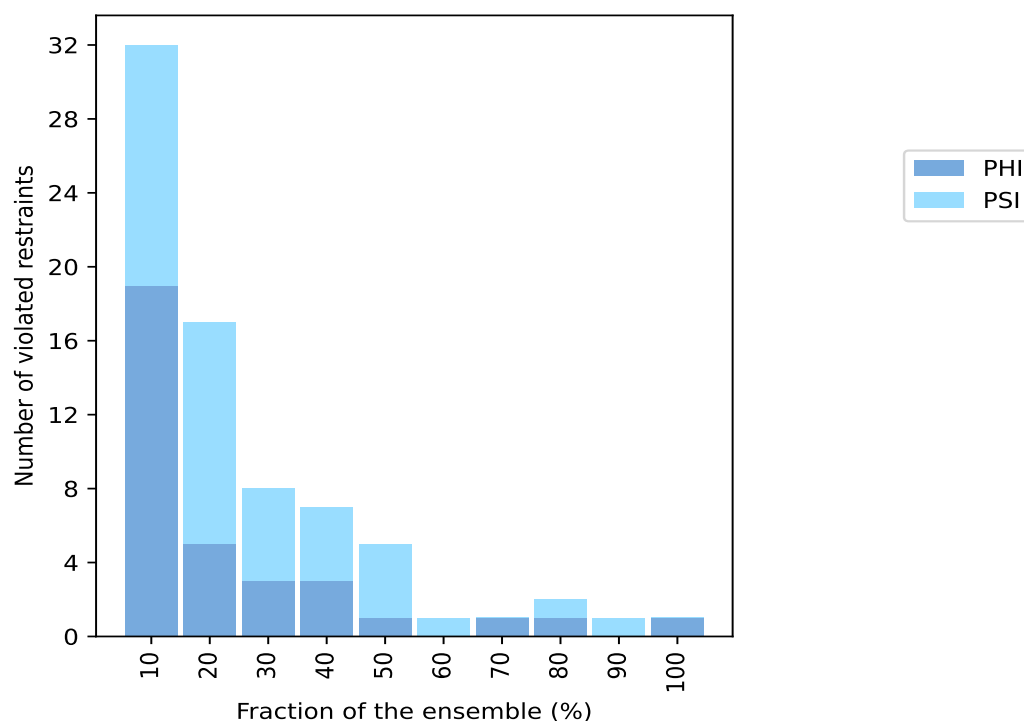
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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>       | %     |
| 19                            | 13  | 32    | 1                        | 10.0  |
| 5                             | 12  | 17    | 2                        | 20.0  |
| 3                             | 5   | 8     | 3                        | 30.0  |
| 3                             | 4   | 7     | 4                        | 40.0  |
| 1                             | 4   | 5     | 5                        | 50.0  |
| 0                             | 1   | 1     | 6                        | 60.0  |
| 1                             | 0   | 1     | 7                        | 70.0  |
| 1                             | 1   | 2     | 8                        | 80.0  |
| 0                             | 1   | 1     | 9                        | 90.0  |
| 1                             | 0   | 1     | 10                       | 100.0 |

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

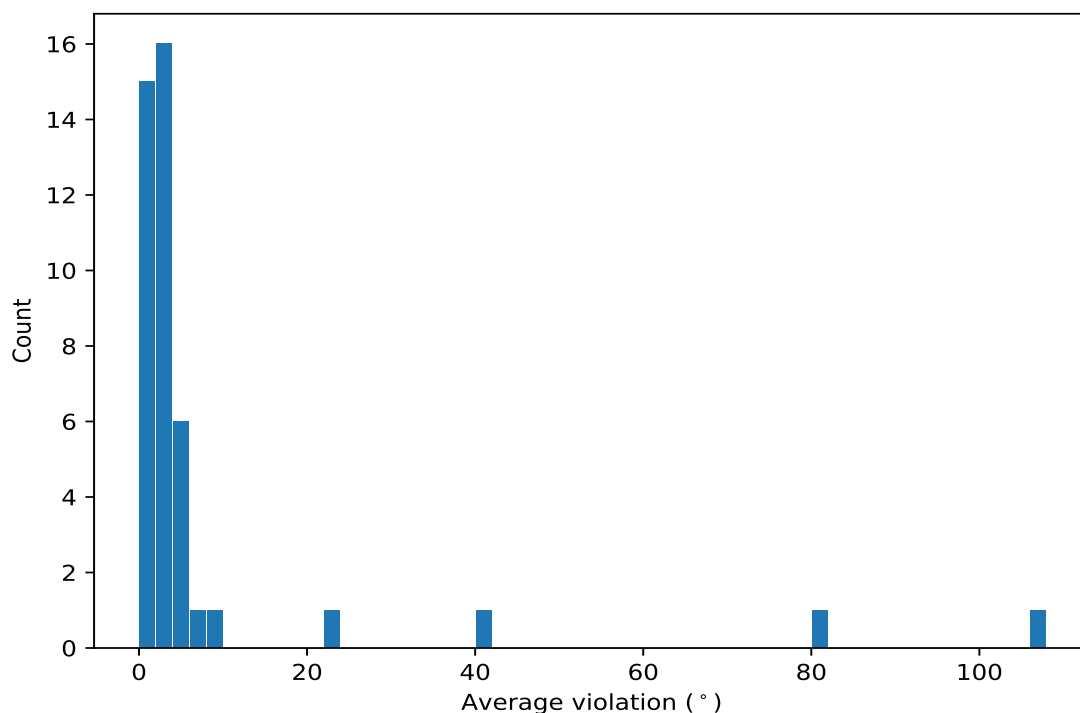
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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 |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,21)  | 1:98:A:ILE:C  | 1:99:A:GLU:N   | 1:99:A:GLU:CA  | 1:99:A:GLU:C  | 10                  | 3.8   | 1.05            | 3.82   |
| (1,206) | 1:109:A:GLN:N | 1:109:A:GLN:CA | 1:109:A:GLN:C  | 1:110:A:ASP:N | 9                   | 4.21  | 1.72            | 3.83   |
| (1,60)  | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:LYS:N  | 8                   | 5.2   | 2.39            | 5.28   |
| (1,17)  | 1:32:A:PHE:C  | 1:33:A:ILE:N   | 1:33:A:ILE:CA  | 1:33:A:ILE:C  | 8                   | 1.89  | 0.67            | 1.78   |
| (1,81)  | 1:44:A:LEU:C  | 1:45:A:SER:N   | 1:45:A:SER:CA  | 1:45:A:SER:C  | 7                   | 1.68  | 0.5             | 1.52   |
| (1,194) | 1:103:A:LYS:N | 1:103:A:LYS:CA | 1:103:A:LYS:C  | 1:104:A:ILE:N | 6                   | 5.23  | 0.91            | 5.25   |
| (1,190) | 1:101:A:GLY:N | 1:101:A:GLY:CA | 1:101:A:GLY:C  | 1:102:A:ASN:N | 5                   | 8.39  | 7.59            | 5.54   |
| (1,189) | 1:100:A:TYR:C | 1:101:A:GLY:N  | 1:101:A:GLY:CA | 1:101:A:GLY:C | 5                   | 7.88  | 6.4             | 5.47   |
| (1,74)  | 1:41:A:THR:N  | 1:41:A:THR:CA  | 1:41:A:THR:C   | 1:42:A:ASN:N  | 5                   | 4.06  | 4.3             | 1.33   |
| (1,192) | 1:102:A:ASN:N | 1:102:A:ASN:CA | 1:102:A:ASN:C  | 1:103:A:LYS:N | 5                   | 2.73  | 1.65            | 2.73   |
| (1,16)  | 1:31:A:GLY:N  | 1:31:A:GLY:CA  | 1:31:A:GLY:C   | 1:32:A:PHE:N  | 5                   | 1.98  | 0.77            | 1.76   |
| (1,220) | 1:116:A:ARG:N | 1:116:A:ARG:CA | 1:116:A:ARG:C  | 1:117:A:VAL:N | 4                   | 81.47 | 46.94           | 102.2  |
| (1,195) | 1:103:A:LYS:C | 1:104:A:ILE:N  | 1:104:A:ILE:CA | 1:104:A:ILE:C | 4                   | 3.51  | 1.15            | 3.86   |

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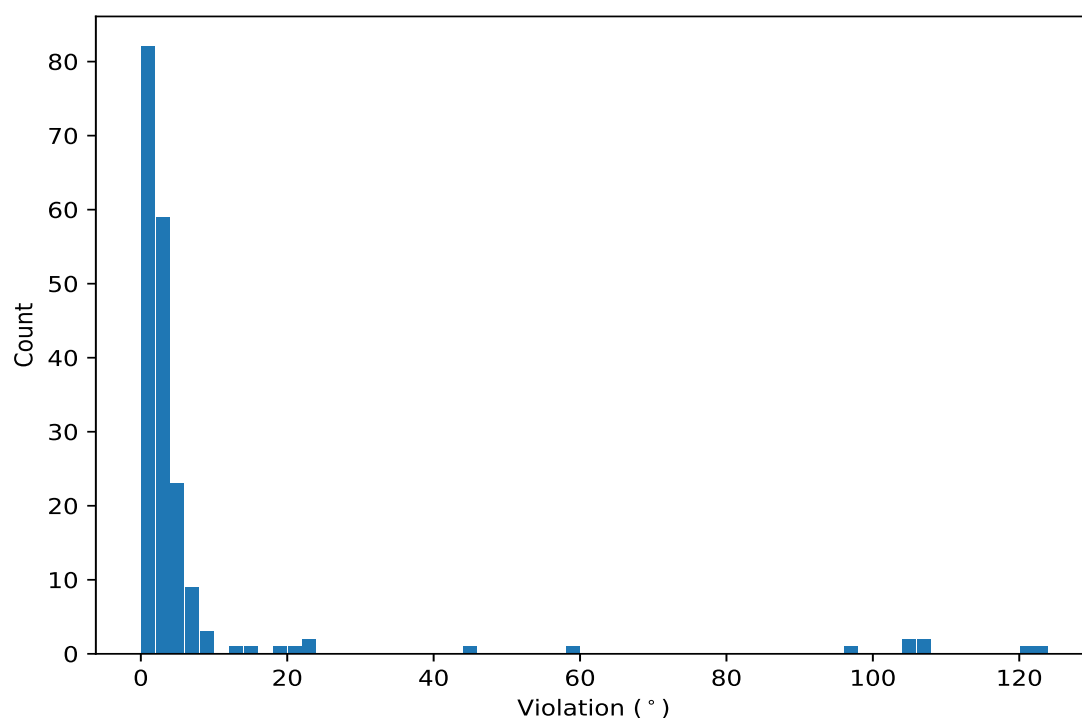
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean   | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|--------|-----------------|--------|
| (1,152) | 1:80:A:SER:N  | 1:80:A:SER:CA  | 1:80:A:SER:C   | 1:81:A:ARG:N  | 4                   | 2.86   | 1.3             | 2.41   |
| (1,14)  | 1:30:A:VAL:N  | 1:30:A:VAL:CA  | 1:30:A:VAL:C   | 1:31:A:GLY:N  | 4                   | 2.26   | 0.87            | 2.26   |
| (1,151) | 1:79:A:GLY:C  | 1:80:A:SER:N   | 1:80:A:SER:CA  | 1:80:A:SER:C  | 4                   | 2.06   | 0.42            | 2.0    |
| (1,107) | 1:57:A:ASP:C  | 1:58:A:LYS:N   | 1:58:A:LYS:CA  | 1:58:A:LYS:C  | 4                   | 2.03   | 0.68            | 2.06   |
| (1,100) | 1:54:A:LEU:N  | 1:54:A:LEU:CA  | 1:54:A:LEU:C   | 1:55:A:GLY:N  | 4                   | 2.02   | 0.52            | 2.13   |
| (1,200) | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C  | 1:107:A:MET:N | 3                   | 41.4   | 45.09           | 18.46  |
| (1,218) | 1:115:A:ASP:N | 1:115:A:ASP:CA | 1:115:A:ASP:C  | 1:116:A:ARG:N | 3                   | 5.68   | 1.85            | 6.54   |
| (1,193) | 1:102:A:ASN:C | 1:103:A:LYS:N  | 1:103:A:LYS:CA | 1:103:A:LYS:C | 3                   | 4.89   | 1.96            | 3.63   |
| (1,181) | 1:95:A:ASP:C  | 1:96:A:GLN:N   | 1:96:A:GLN:CA  | 1:96:A:GLN:C  | 3                   | 2.78   | 0.52            | 2.97   |
| (1,134) | 1:71:A:LYS:N  | 1:71:A:LYS:CA  | 1:71:A:LYS:C   | 1:72:A:GLY:N  | 3                   | 2.71   | 0.99            | 2.68   |
| (1,191) | 1:101:A:GLY:C | 1:102:A:ASN:N  | 1:102:A:ASN:CA | 1:102:A:ASN:C | 3                   | 2.43   | 0.5             | 2.56   |
| (1,174) | 1:92:A:TYR:N  | 1:92:A:TYR:CA  | 1:92:A:TYR:C   | 1:93:A:GLU:N  | 3                   | 1.72   | 0.4             | 1.54   |
| (1,136) | 1:72:A:GLY:N  | 1:72:A:GLY:CA  | 1:72:A:GLY:C   | 1:73:A:PHE:N  | 3                   | 1.28   | 0.26            | 1.19   |
| (1,157) | 1:83:A:ARG:C  | 1:84:A:LEU:N   | 1:84:A:LEU:CA  | 1:84:A:LEU:C  | 2                   | 106.78 | 1.13            | 106.78 |
| (1,156) | 1:83:A:ARG:N  | 1:83:A:ARG:CA  | 1:83:A:ARG:C   | 1:84:A:LEU:N  | 2                   | 23.38  | 22.0            | 23.38  |
| (1,204) | 1:108:A:ILE:N | 1:108:A:ILE:CA | 1:108:A:ILE:C  | 1:109:A:GLN:N | 2                   | 3.65   | 0.55            | 3.65   |
| (1,188) | 1:100:A:TYR:N | 1:100:A:TYR:CA | 1:100:A:TYR:C  | 1:101:A:GLY:N | 2                   | 3.43   | 0.99            | 3.43   |
| (1,212) | 1:112:A:HIS:N | 1:112:A:HIS:CA | 1:112:A:HIS:C  | 1:113:A:LYS:N | 2                   | 2.59   | 0.75            | 2.59   |
| (1,216) | 1:114:A:GLN:N | 1:114:A:GLN:CA | 1:114:A:GLN:C  | 1:115:A:ASP:N | 2                   | 2.39   | 1.29            | 2.39   |
| (1,13)  | 1:29:A:ARG:C  | 1:30:A:VAL:N   | 1:30:A:VAL:CA  | 1:30:A:VAL:C  | 2                   | 2.22   | 0.98            | 2.22   |
| (1,182) | 1:96:A:GLN:N  | 1:96:A:GLN:CA  | 1:96:A:GLN:C   | 1:97:A:SER:N  | 2                   | 1.85   | 0.52            | 1.85   |
| (1,2)   | 1:4:A:MET:N   | 1:4:A:MET:CA   | 1:4:A:MET:C    | 1:5:A:ARG:N   | 2                   | 1.83   | 0.4             | 1.83   |
| (1,162) | 1:86:A:ILE:N  | 1:86:A:ILE:CA  | 1:86:A:ILE:C   | 1:87:A:MET:N  | 2                   | 1.6    | 0.27            | 1.6    |
| (1,173) | 1:91:A:MET:C  | 1:92:A:TYR:N   | 1:92:A:TYR:CA  | 1:92:A:TYR:C  | 2                   | 1.58   | 0.07            | 1.58   |
| (1,208) | 1:110:A:ASP:N | 1:110:A:ASP:CA | 1:110:A:ASP:C  | 1:111:A:LEU:N | 2                   | 1.55   | 0.2             | 1.55   |
| (1,214) | 1:113:A:LYS:N | 1:113:A:LYS:CA | 1:113:A:LYS:C  | 1:114:A:GLN:N | 2                   | 1.27   | 0.01            | 1.27   |
| (1,203) | 1:107:A:MET:C | 1:108:A:ILE:N  | 1:108:A:ILE:CA | 1:108:A:ILE:C | 2                   | 1.26   | 0.15            | 1.26   |
| (1,32)  | 1:11:A:GLU:N  | 1:11:A:GLU:CA  | 1:11:A:GLU:C   | 1:12:A:GLN:N  | 2                   | 1.14   | 0.04            | 1.14   |
| (1,22)  | 1:99:A:GLU:N  | 1:99:A:GLU:CA  | 1:99:A:GLU:C   | 1:100:A:TYR:N | 2                   | 1.06   | 0.01            | 1.06   |
| (1,211) | 1:111:A:LEU:C | 1:112:A:HIS:N  | 1:112:A:HIS:CA | 1:112:A:HIS:C | 2                   | 1.05   | 0.04            | 1.05   |

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

## 10.5 All violated dihedral-angle restraints ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,153) | 1:81:A:ARG:C  | 1:82:A:MET:N   | 1:82:A:MET:CA  | 1:82:A:MET:C  | 7        | 122.43        |
| (1,220) | 1:116:A:ARG:N | 1:116:A:ARG:CA | 1:116:A:ARG:C  | 1:117:A:VAL:N | 7        | 120.05        |
| (1,157) | 1:83:A:ARG:C  | 1:84:A:LEU:N   | 1:84:A:LEU:CA  | 1:84:A:LEU:C  | 2        | 107.91        |
| (1,220) | 1:116:A:ARG:N | 1:116:A:ARG:CA | 1:116:A:ARG:C  | 1:117:A:VAL:N | 6        | 107.71        |
| (1,157) | 1:83:A:ARG:C  | 1:84:A:LEU:N   | 1:84:A:LEU:CA  | 1:84:A:LEU:C  | 5        | 105.64        |
| (1,200) | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C  | 1:107:A:MET:N | 5        | 104.4         |
| (1,220) | 1:116:A:ARG:N | 1:116:A:ARG:CA | 1:116:A:ARG:C  | 1:117:A:VAL:N | 5        | 96.69         |
| (1,219) | 1:115:A:ASP:C | 1:116:A:ARG:N  | 1:116:A:ARG:CA | 1:116:A:ARG:C | 4        | 59.65         |
| (1,156) | 1:83:A:ARG:N  | 1:83:A:ARG:CA  | 1:83:A:ARG:C   | 1:84:A:LEU:N  | 7        | 45.38         |
| (1,154) | 1:82:A:MET:N  | 1:82:A:MET:CA  | 1:82:A:MET:C   | 1:83:A:ARG:N  | 7        | 23.74         |
| (1,190) | 1:101:A:GLY:N | 1:101:A:GLY:CA | 1:101:A:GLY:C  | 1:102:A:ASN:N | 4        | 23.08         |
| (1,189) | 1:100:A:TYR:C | 1:101:A:GLY:N  | 1:101:A:GLY:CA | 1:101:A:GLY:C | 6        | 20.16         |
| (1,200) | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C  | 1:107:A:MET:N | 6        | 18.46         |
| (1,75)  | 1:41:A:THR:C  | 1:42:A:ASN:N   | 1:42:A:ASN:CA  | 1:42:A:ASN:C  | 8        | 14.27         |
| (1,74)  | 1:41:A:THR:N  | 1:41:A:THR:CA  | 1:41:A:THR:C   | 1:42:A:ASN:N  | 8        | 12.36         |
| (1,62)  | 1:27:A:ASP:N  | 1:27:A:ASP:CA  | 1:27:A:ASP:C   | 1:28:A:PRO:N  | 2        | 8.97          |
| (1,60)  | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:LYS:N  | 6        | 8.59          |
| (1,206) | 1:109:A:GLN:N | 1:109:A:GLN:CA | 1:109:A:GLN:C  | 1:110:A:ASP:N | 5        | 8.16          |
| (1,189) | 1:100:A:TYR:C | 1:101:A:GLY:N  | 1:101:A:GLY:CA | 1:101:A:GLY:C | 7        | 7.76          |
| (1,77)  | 1:42:A:ASN:C  | 1:43:A:ASP:N   | 1:43:A:ASP:CA  | 1:43:A:ASP:C  | 8        | 7.74          |
| (1,190) | 1:101:A:GLY:N | 1:101:A:GLY:CA | 1:101:A:GLY:C  | 1:102:A:ASN:N | 5        | 7.7           |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,60)  | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:LYS:N  | 5        | 7.69          |
| (1,193) | 1:102:A:ASN:C | 1:103:A:LYS:N  | 1:103:A:LYS:CA | 1:103:A:LYS:C | 1        | 7.66          |
| (1,218) | 1:115:A:ASP:N | 1:115:A:ASP:CA | 1:115:A:ASP:C  | 1:116:A:ARG:N | 10       | 7.38          |
| (1,60)  | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:LYS:N  | 8        | 7.38          |
| (1,194) | 1:103:A:LYS:N | 1:103:A:LYS:CA | 1:103:A:LYS:C  | 1:104:A:ILE:N | 2        | 6.73          |
| (1,218) | 1:115:A:ASP:N | 1:115:A:ASP:CA | 1:115:A:ASP:C  | 1:116:A:ARG:N | 7        | 6.54          |
| (1,158) | 1:84:A:LEU:N  | 1:84:A:LEU:CA  | 1:84:A:LEU:C   | 1:85:A:ARG:N  | 10       | 5.85          |
| (1,192) | 1:102:A:ASN:N | 1:102:A:ASN:CA | 1:102:A:ASN:C  | 1:103:A:LYS:N | 1        | 5.74          |
| (1,194) | 1:103:A:LYS:N | 1:103:A:LYS:CA | 1:103:A:LYS:C  | 1:104:A:ILE:N | 6        | 5.72          |
| (1,194) | 1:103:A:LYS:N | 1:103:A:LYS:CA | 1:103:A:LYS:C  | 1:104:A:ILE:N | 5        | 5.7           |
| (1,21)  | 1:98:A:ILE:C  | 1:99:A:GLU:N   | 1:99:A:GLU:CA  | 1:99:A:GLU:C  | 3        | 5.56          |
| (1,190) | 1:101:A:GLY:N | 1:101:A:GLY:CA | 1:101:A:GLY:C  | 1:102:A:ASN:N | 2        | 5.54          |
| (1,189) | 1:100:A:TYR:C | 1:101:A:GLY:N  | 1:101:A:GLY:CA | 1:101:A:GLY:C | 5        | 5.47          |
| (1,60)  | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:LYS:N  | 4        | 5.42          |
| (1,206) | 1:109:A:GLN:N | 1:109:A:GLN:CA | 1:109:A:GLN:C  | 1:110:A:ASP:N | 7        | 5.25          |
| (1,60)  | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:LYS:N  | 9        | 5.15          |
| (1,21)  | 1:98:A:ILE:C  | 1:99:A:GLU:N   | 1:99:A:GLU:CA  | 1:99:A:GLU:C  | 1        | 5.03          |
| (1,152) | 1:80:A:SER:N  | 1:80:A:SER:CA  | 1:80:A:SER:C   | 1:81:A:ARG:N  | 5        | 4.97          |
| (1,206) | 1:109:A:GLN:N | 1:109:A:GLN:CA | 1:109:A:GLN:C  | 1:110:A:ASP:N | 1        | 4.81          |
| (1,194) | 1:103:A:LYS:N | 1:103:A:LYS:CA | 1:103:A:LYS:C  | 1:104:A:ILE:N | 4        | 4.8           |
| (1,21)  | 1:98:A:ILE:C  | 1:99:A:GLU:N   | 1:99:A:GLU:CA  | 1:99:A:GLU:C  | 2        | 4.6           |
| (1,195) | 1:103:A:LYS:C | 1:104:A:ILE:N  | 1:104:A:ILE:CA | 1:104:A:ILE:C | 2        | 4.59          |
| (1,206) | 1:109:A:GLN:N | 1:109:A:GLN:CA | 1:109:A:GLN:C  | 1:110:A:ASP:N | 6        | 4.55          |
| (1,195) | 1:103:A:LYS:C | 1:104:A:ILE:N  | 1:104:A:ILE:CA | 1:104:A:ILE:C | 4        | 4.46          |
| (1,188) | 1:100:A:TYR:N | 1:100:A:TYR:CA | 1:100:A:TYR:C  | 1:101:A:GLY:N | 3        | 4.42          |
| (1,194) | 1:103:A:LYS:N | 1:103:A:LYS:CA | 1:103:A:LYS:C  | 1:104:A:ILE:N | 1        | 4.32          |
| (1,204) | 1:108:A:ILE:N | 1:108:A:ILE:CA | 1:108:A:ILE:C  | 1:109:A:GLN:N | 7        | 4.2           |
| (1,74)  | 1:41:A:THR:N  | 1:41:A:THR:CA  | 1:41:A:THR:C   | 1:42:A:ASN:N  | 3        | 4.16          |
| (1,194) | 1:103:A:LYS:N | 1:103:A:LYS:CA | 1:103:A:LYS:C  | 1:104:A:ILE:N | 9        | 4.1           |
| (1,21)  | 1:98:A:ILE:C  | 1:99:A:GLU:N   | 1:99:A:GLU:CA  | 1:99:A:GLU:C  | 4        | 3.99          |
| (1,134) | 1:71:A:LYS:N  | 1:71:A:LYS:CA  | 1:71:A:LYS:C   | 1:72:A:GLY:N  | 10       | 3.93          |
| (1,21)  | 1:98:A:ILE:C  | 1:99:A:GLU:N   | 1:99:A:GLU:CA  | 1:99:A:GLU:C  | 10       | 3.85          |
| (1,206) | 1:109:A:GLN:N | 1:109:A:GLN:CA | 1:109:A:GLN:C  | 1:110:A:ASP:N | 4        | 3.83          |
| (1,21)  | 1:98:A:ILE:C  | 1:99:A:GLU:N   | 1:99:A:GLU:CA  | 1:99:A:GLU:C  | 8        | 3.79          |
| (1,216) | 1:114:A:GLN:N | 1:114:A:GLN:CA | 1:114:A:GLN:C  | 1:115:A:ASP:N | 10       | 3.68          |
| (1,190) | 1:101:A:GLY:N | 1:101:A:GLY:CA | 1:101:A:GLY:C  | 1:102:A:ASN:N | 7        | 3.67          |
| (1,206) | 1:109:A:GLN:N | 1:109:A:GLN:CA | 1:109:A:GLN:C  | 1:110:A:ASP:N | 2        | 3.64          |
| (1,193) | 1:102:A:ASN:C | 1:103:A:LYS:N  | 1:103:A:LYS:CA | 1:103:A:LYS:C | 2        | 3.63          |
| (1,189) | 1:100:A:TYR:C | 1:101:A:GLY:N  | 1:101:A:GLY:CA | 1:101:A:GLY:C | 4        | 3.51          |
| (1,21)  | 1:98:A:ILE:C  | 1:99:A:GLU:N   | 1:99:A:GLU:CA  | 1:99:A:GLU:C  | 5        | 3.43          |
| (1,193) | 1:102:A:ASN:C | 1:103:A:LYS:N  | 1:103:A:LYS:CA | 1:103:A:LYS:C | 4        | 3.39          |
| (1,21)  | 1:98:A:ILE:C  | 1:99:A:GLU:N   | 1:99:A:GLU:CA  | 1:99:A:GLU:C  | 7        | 3.35          |
| (1,212) | 1:112:A:HIS:N | 1:112:A:HIS:CA | 1:112:A:HIS:C  | 1:113:A:LYS:N | 2        | 3.34          |
| (1,14)  | 1:30:A:VAL:N  | 1:30:A:VAL:CA  | 1:30:A:VAL:C   | 1:31:A:GLY:N  | 5        | 3.33          |
| (1,181) | 1:95:A:ASP:C  | 1:96:A:GLN:N   | 1:96:A:GLN:CA  | 1:96:A:GLN:C  | 5        | 3.31          |
| (1,16)  | 1:31:A:GLY:N  | 1:31:A:GLY:CA  | 1:31:A:GLY:C   | 1:32:A:PHE:N  | 7        | 3.29          |
| (1,195) | 1:103:A:LYS:C | 1:104:A:ILE:N  | 1:104:A:ILE:CA | 1:104:A:ILE:C | 1        | 3.27          |
| (1,206) | 1:109:A:GLN:N | 1:109:A:GLN:CA | 1:109:A:GLN:C  | 1:110:A:ASP:N | 3        | 3.23          |
| (1,13)  | 1:29:A:ARG:C  | 1:30:A:VAL:N   | 1:30:A:VAL:CA  | 1:30:A:VAL:C  | 9        | 3.2           |
| (1,17)  | 1:32:A:PHE:C  | 1:33:A:ILE:N   | 1:33:A:ILE:CA  | 1:33:A:ILE:C  | 5        | 3.19          |
| (1,73)  | 1:40:A:LEU:C  | 1:41:A:THR:N   | 1:41:A:THR:CA  | 1:41:A:THR:C  | 8        | 3.17          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,218) | 1:115:A:ASP:N | 1:115:A:ASP:CA | 1:115:A:ASP:C  | 1:116:A:ARG:N | 4        | 3.11          |
| (1,204) | 1:108:A:ILE:N | 1:108:A:ILE:CA | 1:108:A:ILE:C  | 1:109:A:GLN:N | 5        | 3.1           |
| (1,72)  | 1:40:A:LEU:N  | 1:40:A:LEU:CA  | 1:40:A:LEU:C   | 1:41:A:THR:N  | 8        | 3.07          |
| (1,191) | 1:101:A:GLY:C | 1:102:A:ASN:N  | 1:102:A:ASN:CA | 1:102:A:ASN:C | 1        | 2.97          |
| (1,181) | 1:95:A:ASP:C  | 1:96:A:GLN:N   | 1:96:A:GLN:CA  | 1:96:A:GLN:C  | 8        | 2.97          |
| (1,107) | 1:57:A:ASP:C  | 1:58:A:LYS:N   | 1:58:A:LYS:CA  | 1:58:A:LYS:C  | 7        | 2.94          |
| (1,60)  | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:LYS:N  | 3        | 2.91          |
| (1,14)  | 1:30:A:VAL:N  | 1:30:A:VAL:CA  | 1:30:A:VAL:C   | 1:31:A:GLY:N  | 10       | 2.89          |
| (1,152) | 1:80:A:SER:N  | 1:80:A:SER:CA  | 1:80:A:SER:C   | 1:81:A:ARG:N  | 2        | 2.85          |
| (1,81)  | 1:44:A:LEU:C  | 1:45:A:SER:N   | 1:45:A:SER:CA  | 1:45:A:SER:C  | 5        | 2.8           |
| (1,192) | 1:102:A:ASN:N | 1:102:A:ASN:CA | 1:102:A:ASN:C  | 1:103:A:LYS:N | 2        | 2.73          |
| (1,192) | 1:102:A:ASN:N | 1:102:A:ASN:CA | 1:102:A:ASN:C  | 1:103:A:LYS:N | 4        | 2.73          |
| (1,151) | 1:79:A:GLY:C  | 1:80:A:SER:N   | 1:80:A:SER:CA  | 1:80:A:SER:C  | 8        | 2.69          |
| (1,134) | 1:71:A:LYS:N  | 1:71:A:LYS:CA  | 1:71:A:LYS:C   | 1:72:A:GLY:N  | 4        | 2.68          |
| (1,60)  | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:LYS:N  | 7        | 2.65          |
| (1,100) | 1:54:A:LEU:N  | 1:54:A:LEU:CA  | 1:54:A:LEU:C   | 1:55:A:GLY:N  | 6        | 2.59          |
| (1,21)  | 1:98:A:ILE:C  | 1:99:A:GLU:N   | 1:99:A:GLU:CA  | 1:99:A:GLU:C  | 9        | 2.58          |
| (1,213) | 1:112:A:HIS:C | 1:113:A:LYS:N  | 1:113:A:LYS:CA | 1:113:A:LYS:C | 5        | 2.56          |
| (1,191) | 1:101:A:GLY:C | 1:102:A:ASN:N  | 1:102:A:ASN:CA | 1:102:A:ASN:C | 10       | 2.56          |
| (1,189) | 1:100:A:TYR:C | 1:101:A:GLY:N  | 1:101:A:GLY:CA | 1:101:A:GLY:C | 9        | 2.5           |
| (1,188) | 1:100:A:TYR:N | 1:100:A:TYR:CA | 1:100:A:TYR:C  | 1:101:A:GLY:N | 8        | 2.44          |
| (1,100) | 1:54:A:LEU:N  | 1:54:A:LEU:CA  | 1:54:A:LEU:C   | 1:55:A:GLY:N  | 5        | 2.38          |
| (1,17)  | 1:32:A:PHE:C  | 1:33:A:ILE:N   | 1:33:A:ILE:CA  | 1:33:A:ILE:C  | 2        | 2.38          |
| (1,182) | 1:96:A:GLN:N  | 1:96:A:GLN:CA  | 1:96:A:GLN:C   | 1:97:A:SER:N  | 8        | 2.37          |
| (1,206) | 1:109:A:GLN:N | 1:109:A:GLN:CA | 1:109:A:GLN:C  | 1:110:A:ASP:N | 10       | 2.35          |
| (1,16)  | 1:31:A:GLY:N  | 1:31:A:GLY:CA  | 1:31:A:GLY:C   | 1:32:A:PHE:N  | 8        | 2.34          |
| (1,76)  | 1:42:A:ASN:N  | 1:42:A:ASN:CA  | 1:42:A:ASN:C   | 1:43:A:ASP:N  | 8        | 2.32          |
| (1,174) | 1:92:A:TYR:N  | 1:92:A:TYR:CA  | 1:92:A:TYR:C   | 1:93:A:GLU:N  | 9        | 2.27          |
| (1,17)  | 1:32:A:PHE:C  | 1:33:A:ILE:N   | 1:33:A:ILE:CA  | 1:33:A:ILE:C  | 7        | 2.27          |
| (1,107) | 1:57:A:ASP:C  | 1:58:A:LYS:N   | 1:58:A:LYS:CA  | 1:58:A:LYS:C  | 5        | 2.26          |
| (1,2)   | 1:4:A:MET:N   | 1:4:A:MET:CA   | 1:4:A:MET:C    | 1:5:A:ARG:N   | 3        | 2.22          |
| (1,142) | 1:75:A:LYS:N  | 1:75:A:LYS:CA  | 1:75:A:LYS:C   | 1:76:A:SER:N  | 10       | 2.17          |
| (1,215) | 1:113:A:LYS:C | 1:114:A:GLN:N  | 1:114:A:GLN:CA | 1:114:A:GLN:C | 10       | 2.12          |
| (1,151) | 1:79:A:GLY:C  | 1:80:A:SER:N   | 1:80:A:SER:CA  | 1:80:A:SER:C  | 6        | 2.11          |
| (1,181) | 1:95:A:ASP:C  | 1:96:A:GLN:N   | 1:96:A:GLN:CA  | 1:96:A:GLN:C  | 9        | 2.07          |
| (1,206) | 1:109:A:GLN:N | 1:109:A:GLN:CA | 1:109:A:GLN:C  | 1:110:A:ASP:N | 9        | 2.06          |
| (1,84)  | 1:46:A:GLN:N  | 1:46:A:GLN:CA  | 1:46:A:GLN:C   | 1:47:A:ALA:N  | 8        | 2.05          |
| (1,152) | 1:80:A:SER:N  | 1:80:A:SER:CA  | 1:80:A:SER:C   | 1:81:A:ARG:N  | 1        | 1.97          |
| (1,190) | 1:101:A:GLY:N | 1:101:A:GLY:CA | 1:101:A:GLY:C  | 1:102:A:ASN:N | 1        | 1.94          |
| (1,151) | 1:79:A:GLY:C  | 1:80:A:SER:N   | 1:80:A:SER:CA  | 1:80:A:SER:C  | 10       | 1.9           |
| (1,162) | 1:86:A:ILE:N  | 1:86:A:ILE:CA  | 1:86:A:ILE:C   | 1:87:A:MET:N  | 5        | 1.88          |
| (1,100) | 1:54:A:LEU:N  | 1:54:A:LEU:CA  | 1:54:A:LEU:C   | 1:55:A:GLY:N  | 2        | 1.88          |
| (1,107) | 1:57:A:ASP:C  | 1:58:A:LYS:N   | 1:58:A:LYS:CA  | 1:58:A:LYS:C  | 10       | 1.86          |
| (1,212) | 1:112:A:HIS:N | 1:112:A:HIS:CA | 1:112:A:HIS:C  | 1:113:A:LYS:N | 9        | 1.84          |
| (1,21)  | 1:98:A:ILE:C  | 1:99:A:GLU:N   | 1:99:A:GLU:CA  | 1:99:A:GLU:C  | 6        | 1.84          |
| (1,17)  | 1:32:A:PHE:C  | 1:33:A:ILE:N   | 1:33:A:ILE:CA  | 1:33:A:ILE:C  | 9        | 1.82          |
| (1,185) | 1:97:A:SER:C  | 1:98:A:ILE:N   | 1:98:A:ILE:CA  | 1:98:A:ILE:C  | 2        | 1.8           |
| (1,60)  | 1:25:A:VAL:N  | 1:25:A:VAL:CA  | 1:25:A:VAL:C   | 1:26:A:LYS:N  | 10       | 1.8           |
| (1,81)  | 1:44:A:LEU:C  | 1:45:A:SER:N   | 1:45:A:SER:CA  | 1:45:A:SER:C  | 4        | 1.79          |
| (1,191) | 1:101:A:GLY:C | 1:102:A:ASN:N  | 1:102:A:ASN:CA | 1:102:A:ASN:C | 3        | 1.76          |
| (1,16)  | 1:31:A:GLY:N  | 1:31:A:GLY:CA  | 1:31:A:GLY:C   | 1:32:A:PHE:N  | 6        | 1.76          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,208) | 1:110:A:ASP:N | 1:110:A:ASP:CA | 1:110:A:ASP:C  | 1:111:A:LEU:N | 9        | 1.75          |
| (1,17)  | 1:32:A:PHE:C  | 1:33:A:ILE:N   | 1:33:A:ILE:CA  | 1:33:A:ILE:C  | 10       | 1.75          |
| (1,195) | 1:103:A:LYS:C | 1:104:A:ILE:N  | 1:104:A:ILE:CA | 1:104:A:ILE:C | 5        | 1.72          |
| (1,59)  | 1:24:A:LYS:C  | 1:25:A:VAL:N   | 1:25:A:VAL:CA  | 1:25:A:VAL:C  | 6        | 1.72          |
| (1,148) | 1:78:A:LEU:N  | 1:78:A:LEU:CA  | 1:78:A:LEU:C   | 1:79:A:GLY:N  | 10       | 1.67          |
| (1,173) | 1:91:A:MET:C  | 1:92:A:TYR:N   | 1:92:A:TYR:CA  | 1:92:A:TYR:C  | 1        | 1.65          |
| (1,152) | 1:80:A:SER:N  | 1:80:A:SER:CA  | 1:80:A:SER:C   | 1:81:A:ARG:N  | 10       | 1.65          |
| (1,136) | 1:72:A:GLY:N  | 1:72:A:GLY:CA  | 1:72:A:GLY:C   | 1:73:A:PHE:N  | 1        | 1.64          |
| (1,81)  | 1:44:A:LEU:C  | 1:45:A:SER:N   | 1:45:A:SER:CA  | 1:45:A:SER:C  | 7        | 1.63          |
| (1,14)  | 1:30:A:VAL:N  | 1:30:A:VAL:CA  | 1:30:A:VAL:C   | 1:31:A:GLY:N  | 8        | 1.63          |
| (1,17)  | 1:32:A:PHE:C  | 1:33:A:ILE:N   | 1:33:A:ILE:CA  | 1:33:A:ILE:C  | 4        | 1.55          |
| (1,174) | 1:92:A:TYR:N  | 1:92:A:TYR:CA  | 1:92:A:TYR:C   | 1:93:A:GLU:N  | 7        | 1.54          |
| (1,155) | 1:82:A:MET:C  | 1:83:A:ARG:N   | 1:83:A:ARG:CA  | 1:83:A:ARG:C  | 10       | 1.53          |
| (1,89)  | 1:48:A:LYS:C  | 1:49:A:VAL:N   | 1:49:A:VAL:CA  | 1:49:A:VAL:C  | 5        | 1.53          |
| (1,151) | 1:79:A:GLY:C  | 1:80:A:SER:N   | 1:80:A:SER:CA  | 1:80:A:SER:C  | 9        | 1.52          |
| (1,81)  | 1:44:A:LEU:C  | 1:45:A:SER:N   | 1:45:A:SER:CA  | 1:45:A:SER:C  | 2        | 1.52          |
| (1,173) | 1:91:A:MET:C  | 1:92:A:TYR:N   | 1:92:A:TYR:CA  | 1:92:A:TYR:C  | 8        | 1.51          |
| (1,134) | 1:71:A:LYS:N  | 1:71:A:LYS:CA  | 1:71:A:LYS:C   | 1:72:A:GLY:N  | 3        | 1.51          |
| (1,81)  | 1:44:A:LEU:C  | 1:45:A:SER:N   | 1:45:A:SER:CA  | 1:45:A:SER:C  | 1        | 1.47          |
| (1,63)  | 1:28:A:PRO:C  | 1:29:A:ARG:N   | 1:29:A:ARG:CA  | 1:29:A:ARG:C  | 1        | 1.47          |
| (1,81)  | 1:44:A:LEU:C  | 1:45:A:SER:N   | 1:45:A:SER:CA  | 1:45:A:SER:C  | 9        | 1.45          |
| (1,178) | 1:94:A:TYR:N  | 1:94:A:TYR:CA  | 1:94:A:TYR:C   | 1:95:A:ASP:N  | 2        | 1.44          |
| (1,220) | 1:116:A:ARG:N | 1:116:A:ARG:CA | 1:116:A:ARG:C  | 1:117:A:VAL:N | 9        | 1.43          |
| (1,2)   | 1:4:A:MET:N   | 1:4:A:MET:CA   | 1:4:A:MET:C    | 1:5:A:ARG:N   | 4        | 1.43          |
| (1,203) | 1:107:A:MET:C | 1:108:A:ILE:N  | 1:108:A:ILE:CA | 1:108:A:ILE:C | 1        | 1.41          |
| (1,156) | 1:83:A:ARG:N  | 1:83:A:ARG:CA  | 1:83:A:ARG:C   | 1:84:A:LEU:N  | 1        | 1.38          |
| (1,208) | 1:110:A:ASP:N | 1:110:A:ASP:CA | 1:110:A:ASP:C  | 1:111:A:LEU:N | 7        | 1.35          |
| (1,18)  | 1:33:A:ILE:N  | 1:33:A:ILE:CA  | 1:33:A:ILE:C   | 1:34:A:THR:N  | 1        | 1.35          |
| (1,200) | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C  | 1:107:A:MET:N | 9        | 1.34          |
| (1,174) | 1:92:A:TYR:N  | 1:92:A:TYR:CA  | 1:92:A:TYR:C   | 1:93:A:GLU:N  | 6        | 1.34          |
| (1,182) | 1:96:A:GLN:N  | 1:96:A:GLN:CA  | 1:96:A:GLN:C   | 1:97:A:SER:N  | 6        | 1.33          |
| (1,162) | 1:86:A:ILE:N  | 1:86:A:ILE:CA  | 1:86:A:ILE:C   | 1:87:A:MET:N  | 4        | 1.33          |
| (1,74)  | 1:41:A:THR:N  | 1:41:A:THR:CA  | 1:41:A:THR:C   | 1:42:A:ASN:N  | 4        | 1.33          |
| (1,74)  | 1:41:A:THR:N  | 1:41:A:THR:CA  | 1:41:A:THR:C   | 1:42:A:ASN:N  | 5        | 1.33          |
| (1,16)  | 1:31:A:GLY:N  | 1:31:A:GLY:CA  | 1:31:A:GLY:C   | 1:32:A:PHE:N  | 4        | 1.29          |
| (1,214) | 1:113:A:LYS:N | 1:113:A:LYS:CA | 1:113:A:LYS:C  | 1:114:A:GLN:N | 5        | 1.28          |
| (1,192) | 1:102:A:ASN:N | 1:102:A:ASN:CA | 1:102:A:ASN:C  | 1:103:A:LYS:N | 9        | 1.28          |
| (1,214) | 1:113:A:LYS:N | 1:113:A:LYS:CA | 1:113:A:LYS:C  | 1:114:A:GLN:N | 1        | 1.27          |
| (1,12)  | 1:28:A:PRO:N  | 1:28:A:PRO:CA  | 1:28:A:PRO:C   | 1:29:A:ARG:N  | 1        | 1.26          |
| (1,100) | 1:54:A:LEU:N  | 1:54:A:LEU:CA  | 1:54:A:LEU:C   | 1:55:A:GLY:N  | 8        | 1.25          |
| (1,13)  | 1:29:A:ARG:C  | 1:30:A:VAL:N   | 1:30:A:VAL:CA  | 1:30:A:VAL:C  | 8        | 1.25          |
| (1,141) | 1:74:A:ILE:C  | 1:75:A:LYS:N   | 1:75:A:LYS:CA  | 1:75:A:LYS:C  | 4        | 1.23          |
| (1,16)  | 1:31:A:GLY:N  | 1:31:A:GLY:CA  | 1:31:A:GLY:C   | 1:32:A:PHE:N  | 10       | 1.21          |
| (1,87)  | 1:47:A:ALA:C  | 1:48:A:LYS:N   | 1:48:A:LYS:CA  | 1:48:A:LYS:C  | 10       | 1.2           |
| (1,14)  | 1:30:A:VAL:N  | 1:30:A:VAL:CA  | 1:30:A:VAL:C   | 1:31:A:GLY:N  | 9        | 1.2           |
| (1,136) | 1:72:A:GLY:N  | 1:72:A:GLY:CA  | 1:72:A:GLY:C   | 1:73:A:PHE:N  | 5        | 1.19          |
| (1,32)  | 1:11:A:GLU:N  | 1:11:A:GLU:CA  | 1:11:A:GLU:C   | 1:12:A:GLN:N  | 1        | 1.19          |
| (1,23)  | 1:2:A:SER:C   | 1:3:A:SER:N    | 1:3:A:SER:CA   | 1:3:A:SER:C   | 3        | 1.18          |
| (1,83)  | 1:45:A:SER:C  | 1:46:A:GLN:N   | 1:46:A:GLN:CA  | 1:46:A:GLN:C  | 8        | 1.17          |
| (1,192) | 1:102:A:ASN:N | 1:102:A:ASN:CA | 1:102:A:ASN:C  | 1:103:A:LYS:N | 6        | 1.15          |
| (1,159) | 1:84:A:LEU:C  | 1:85:A:ARG:N   | 1:85:A:ARG:CA  | 1:85:A:ARG:C  | 10       | 1.15          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1)   | 1:3:A:SER:C   | 1:4:A:MET:N    | 1:4:A:MET:CA   | 1:4:A:MET:C   | 5        | 1.12          |
| (1,203) | 1:107:A:MET:C | 1:108:A:ILE:N  | 1:108:A:ILE:CA | 1:108:A:ILE:C | 10       | 1.11          |
| (1,74)  | 1:41:A:THR:N  | 1:41:A:THR:CA  | 1:41:A:THR:C   | 1:42:A:ASN:N  | 10       | 1.11          |
| (1,216) | 1:114:A:GLN:N | 1:114:A:GLN:CA | 1:114:A:GLN:C  | 1:115:A:ASP:N | 1        | 1.1           |
| (1,32)  | 1:11:A:GLU:N  | 1:11:A:GLU:CA  | 1:11:A:GLU:C   | 1:12:A:GLN:N  | 7        | 1.1           |
| (1,211) | 1:111:A:LEU:C | 1:112:A:HIS:N  | 1:112:A:HIS:CA | 1:112:A:HIS:C | 1        | 1.09          |
| (1,132) | 1:70:A:ALA:N  | 1:70:A:ALA:CA  | 1:70:A:ALA:C   | 1:71:A:LYS:N  | 5        | 1.08          |
| (1,17)  | 1:32:A:PHE:C  | 1:33:A:ILE:N   | 1:33:A:ILE:CA  | 1:33:A:ILE:C  | 8        | 1.08          |
| (1,170) | 1:90:A:LEU:N  | 1:90:A:LEU:CA  | 1:90:A:LEU:C   | 1:91:A:MET:N  | 1        | 1.07          |
| (1,81)  | 1:44:A:LEU:C  | 1:45:A:SER:N   | 1:45:A:SER:CA  | 1:45:A:SER:C  | 6        | 1.07          |
| (1,22)  | 1:99:A:GLU:N  | 1:99:A:GLU:CA  | 1:99:A:GLU:C   | 1:100:A:TYR:N | 3        | 1.07          |
| (1,107) | 1:57:A:ASP:C  | 1:58:A:LYS:N   | 1:58:A:LYS:CA  | 1:58:A:LYS:C  | 8        | 1.05          |
| (1,22)  | 1:99:A:GLU:N  | 1:99:A:GLU:CA  | 1:99:A:GLU:C   | 1:100:A:TYR:N | 9        | 1.05          |
| (1,17)  | 1:32:A:PHE:C  | 1:33:A:ILE:N   | 1:33:A:ILE:CA  | 1:33:A:ILE:C  | 1        | 1.05          |
| (1,136) | 1:72:A:GLY:N  | 1:72:A:GLY:CA  | 1:72:A:GLY:C   | 1:73:A:PHE:N  | 2        | 1.02          |
| (1,211) | 1:111:A:LEU:C | 1:112:A:HIS:N  | 1:112:A:HIS:CA | 1:112:A:HIS:C | 2        | 1.01          |
| (1,201) | 1:106:A:ARG:C | 1:107:A:MET:N  | 1:107:A:MET:CA | 1:107:A:MET:C | 2        | 1.01          |