



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 09:05 AM UTC

PDB ID : 2N6F / pdb\_00002n6f  
BMRB ID : 25762  
Title : Structure of Pleiotrophin  
Authors : Ryan, E.O.; Shen, D.; Wang, X.  
Deposited on : 2015-08-20

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<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

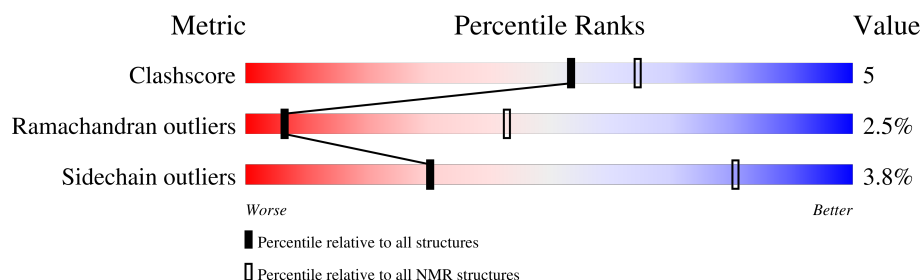
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 77%.

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     | 136    |                  |

## 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: *fewest violations*.

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:16-A:57 (42)        | 1.29              | 3            |
| 2                                    | A:64-A:110 (47)       | 1.80              | 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 3 clusters. No single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 2163 atoms, of which 1098 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Pleiotrophin.

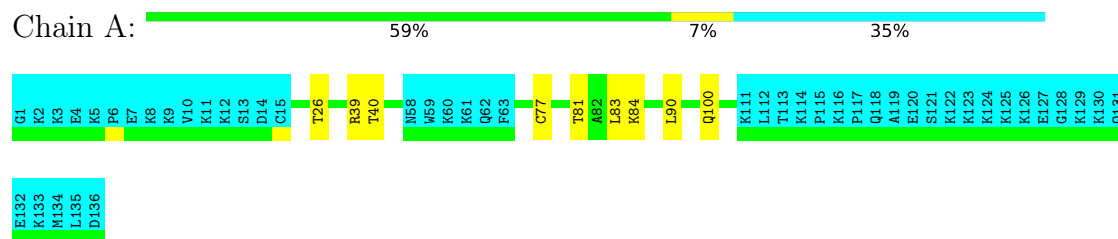
| Mol | Chain | Residues | Atoms |     |      |     |     |    | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|-------|
| 1   | A     | 136      | Total | C   | H    | N   | O   | S  | 0     |
|     |       |          | 2163  | 658 | 1098 | 197 | 198 | 12 |       |

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

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

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

- Molecule 1: Pleiotrophin

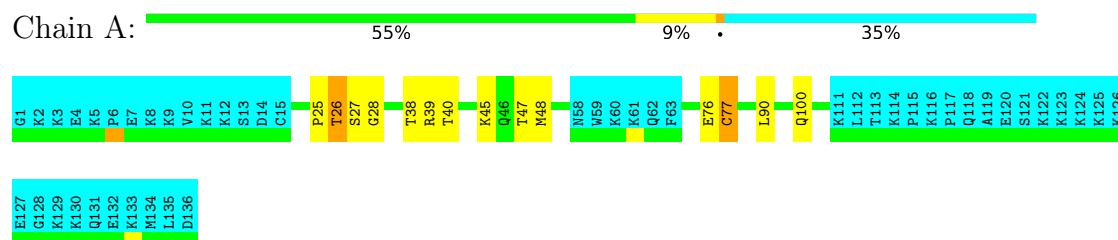


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

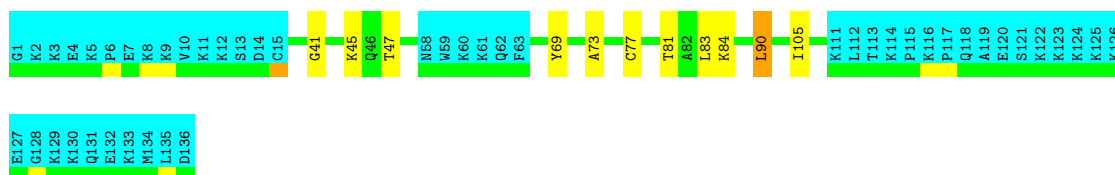
- Molecule 1: Pleiotrophin



#### 4.2.2 Score per residue for model 2

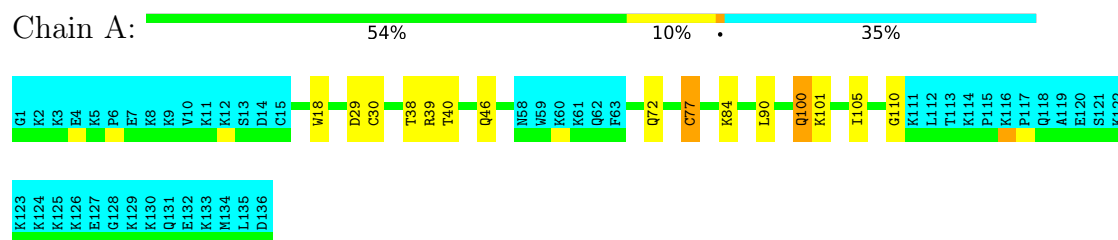
- Molecule 1: Pleiotrophin





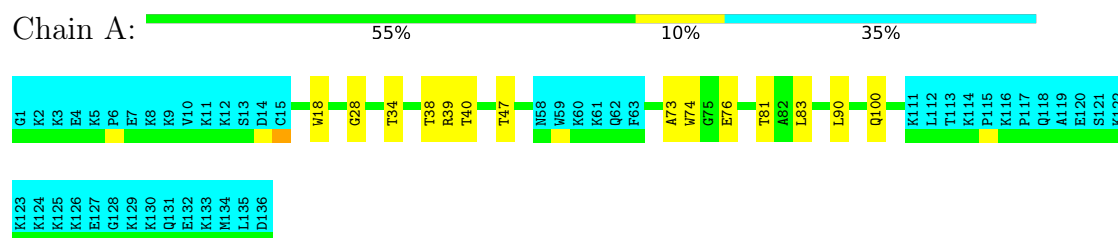
#### 4.2.3 Score per residue for model 3

- Molecule 1: Pleiotrophin



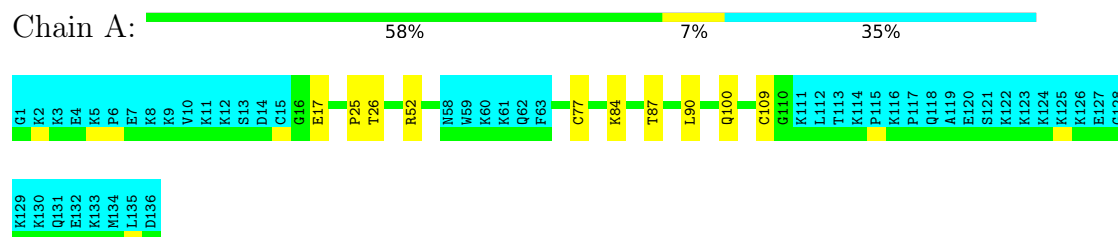
#### 4.2.4 Score per residue for model 4

- Molecule 1: Pleiotrophin



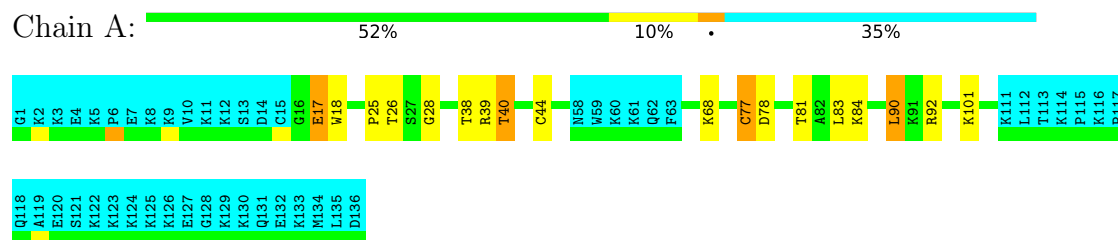
#### 4.2.5 Score per residue for model 5

- Molecule 1: Pleiotrophin



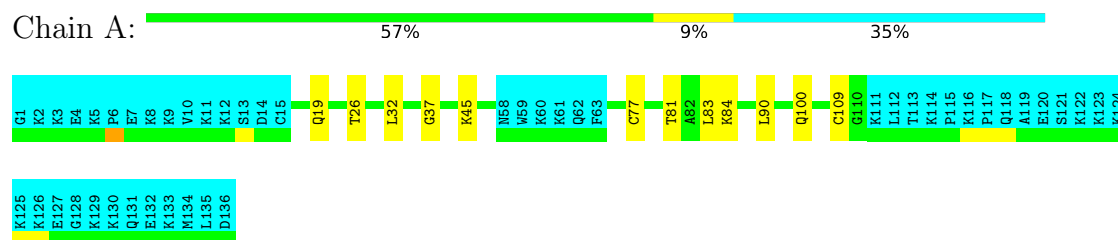
#### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Pleiotrophin



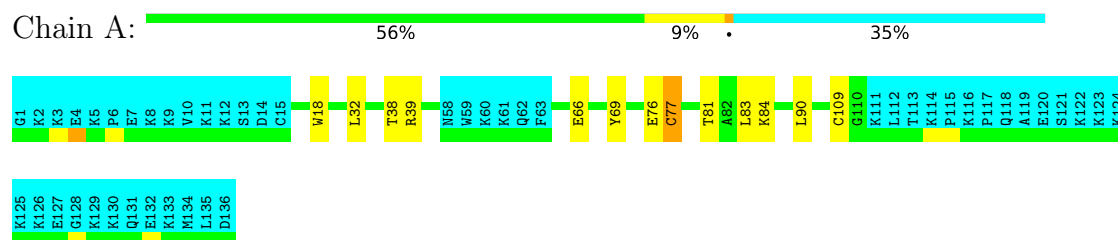
#### 4.2.7 Score per residue for model 7

- Molecule 1: Pleiotrophin



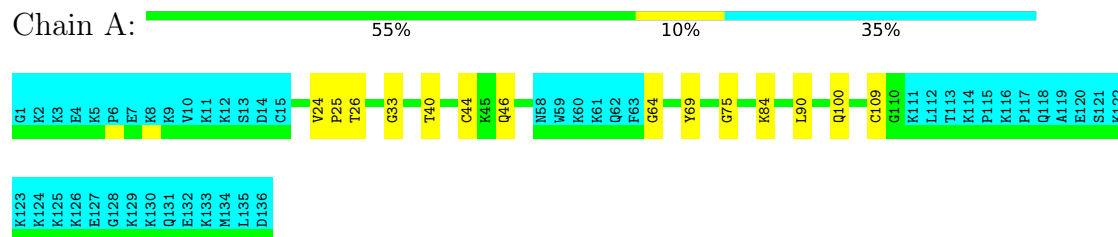
#### 4.2.8 Score per residue for model 8

- Molecule 1: Pleiotrophin



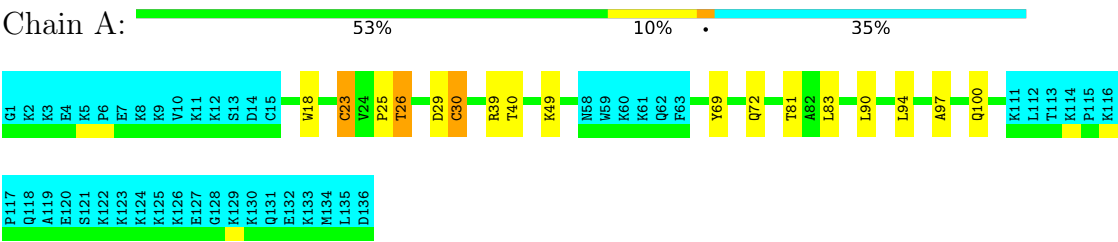
#### 4.2.9 Score per residue for model 9

- Molecule 1: Pleiotrophin



4.2.10 Score per residue for model 10

● Molecule 1: Pleiotrophin





## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

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

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1280           |
| Number of shifts mapped to atoms             | 1280           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 77%            |

## 6 Model quality [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 673   | 656      | 655      | 7±3     |
| All | All   | 6730  | 6560     | 6550     | 69      |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:69:TYR:CE2  | 1:A:90:LEU:HB2  | 0.74     | 2.16        | 2      | 1     |
| 1:A:84:LYS:HB2  | 1:A:109:CYS:SG  | 0.65     | 2.30        | 9      | 4     |
| 1:A:81:THR:O    | 1:A:83:LEU:HG   | 0.60     | 1.96        | 4      | 6     |
| 1:A:68:LYS:O    | 1:A:90:LEU:HA   | 0.60     | 1.95        | 6      | 1     |
| 1:A:90:LEU:HD12 | 1:A:101:LYS:HA  | 0.59     | 1.74        | 6      | 1     |
| 1:A:69:TYR:CE1  | 1:A:90:LEU:HD23 | 0.59     | 2.32        | 8      | 1     |
| 1:A:90:LEU:HB2  | 1:A:100:GLN:O   | 0.59     | 1.96        | 10     | 7     |
| 1:A:25:PRO:O    | 1:A:26:THR:HB   | 0.58     | 1.98        | 10     | 5     |
| 1:A:18:TRP:HA   | 1:A:38:THR:O    | 0.57     | 2.00        | 3      | 4     |
| 1:A:90:LEU:HD13 | 1:A:90:LEU:O    | 0.53     | 2.03        | 6      | 1     |
| 1:A:40:THR:HA   | 1:A:45:LYS:O    | 0.53     | 2.03        | 1      | 1     |
| 1:A:18:TRP:CD2  | 1:A:39:ARG:HB2  | 0.50     | 2.42        | 10     | 4     |
| 1:A:17:GLU:CD   | 1:A:17:GLU:H    | 0.49     | 2.15        | 6      | 1     |
| 1:A:77:CYS:HA   | 1:A:84:LYS:HB3  | 0.48     | 1.84        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:94:LEU:HB2  | 1:A:97:ALA:HB3  | 0.47     | 1.85        | 10     | 1     |
| 1:A:39:ARG:HG2  | 1:A:40:THR:N    | 0.47     | 2.24        | 6      | 3     |
| 1:A:90:LEU:C    | 1:A:90:LEU:HD23 | 0.47     | 2.35        | 1      | 2     |
| 1:A:64:GLY:HA3  | 1:A:69:TYR:CG   | 0.46     | 2.46        | 9      | 1     |
| 1:A:19:GLN:O    | 1:A:37:GLY:HA2  | 0.46     | 2.11        | 7      | 1     |
| 1:A:40:THR:HG22 | 1:A:44:CYS:HA   | 0.45     | 1.89        | 6      | 1     |
| 1:A:69:TYR:CZ   | 1:A:90:LEU:HB2  | 0.45     | 2.47        | 8      | 1     |
| 1:A:38:THR:HG22 | 1:A:48:MET:HB3  | 0.44     | 1.87        | 1      | 1     |
| 1:A:100:GLN:CD  | 1:A:100:GLN:H   | 0.44     | 2.20        | 10     | 2     |
| 1:A:74:TRP:H    | 1:A:74:TRP:CD1  | 0.44     | 2.30        | 4      | 1     |
| 1:A:77:CYS:H    | 1:A:84:LYS:HG3  | 0.44     | 1.73        | 6      | 1     |
| 1:A:25:PRO:O    | 1:A:26:THR:CB   | 0.44     | 2.64        | 10     | 1     |
| 1:A:77:CYS:CA   | 1:A:84:LYS:HB3  | 0.44     | 2.43        | 2      | 1     |
| 1:A:90:LEU:HD13 | 1:A:90:LEU:C    | 0.43     | 2.38        | 4      | 3     |
| 1:A:78:ASP:OD2  | 1:A:81:THR:HG22 | 0.43     | 2.13        | 6      | 1     |
| 1:A:26:THR:HB   | 1:A:32:LEU:O    | 0.42     | 2.14        | 7      | 1     |
| 1:A:69:TYR:CD1  | 1:A:90:LEU:HD23 | 0.42     | 2.50        | 8      | 1     |
| 1:A:90:LEU:C    | 1:A:90:LEU:HD22 | 0.41     | 2.40        | 6      | 1     |
| 1:A:24:VAL:O    | 1:A:33:GLY:HA3  | 0.41     | 2.15        | 9      | 1     |
| 1:A:77:CYS:SG   | 1:A:84:LYS:HG3  | 0.41     | 2.56        | 3      | 1     |
| 1:A:74:TRP:CZ3  | 1:A:76:GLU:HB2  | 0.41     | 2.51        | 4      | 1     |
| 1:A:18:TRP:CE2  | 1:A:39:ARG:HB2  | 0.41     | 2.50        | 3      | 1     |
| 1:A:76:GLU:O    | 1:A:77:CYS:C    | 0.40     | 2.63        | 8      | 2     |
| 1:A:29:ASP:O    | 1:A:30:CYS:HB2  | 0.40     | 2.16        | 10     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed       | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|----------------|--------------|------------|------------|-------------|----|
| 1   | A     | 89/136 (65%)   | 80±2 (90±2%) | 7±2 (8±2%) | 2±1 (2±1%) | 6           | 43 |
| All | All   | 890/1360 (65%) | 798 (90%)    | 70 (8%)    | 22 (2%)    | 6           | 43 |

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 77  | CYS  | 6              |
| 1   | A     | 28  | GLY  | 3              |
| 1   | A     | 26  | THR  | 2              |
| 1   | A     | 73  | ALA  | 2              |
| 1   | A     | 30  | CYS  | 2              |
| 1   | A     | 46  | GLN  | 2              |
| 1   | A     | 27  | SER  | 1              |
| 1   | A     | 110 | GLY  | 1              |
| 1   | A     | 45  | LYS  | 1              |
| 1   | A     | 75  | GLY  | 1              |
| 1   | A     | 23  | CYS  | 1              |

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

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

| Mol | Chain | Analysed       | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|----------------|--------------|------------|-------------|----|
| 1   | A     | 73/117 (62%)   | 70±1 (96±2%) | 3±1 (4±2%) | 30          | 81 |
| All | All   | 730/1170 (62%) | 702 (96%)    | 28 (4%)    | 30          | 81 |

All 19 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     | 40  | THR  | 4              |
| 1   | A     | 47  | THR  | 3              |
| 1   | A     | 90  | LEU  | 2              |
| 1   | A     | 105 | ILE  | 2              |
| 1   | A     | 72  | GLN  | 2              |
| 1   | A     | 17  | GLU  | 2              |
| 1   | A     | 45  | LYS  | 1              |
| 1   | A     | 100 | GLN  | 1              |
| 1   | A     | 101 | LYS  | 1              |
| 1   | A     | 34  | THR  | 1              |
| 1   | A     | 52  | ARG  | 1              |
| 1   | A     | 87  | THR  | 1              |
| 1   | A     | 92  | ARG  | 1              |
| 1   | A     | 32  | LEU  | 1              |
| 1   | A     | 66  | GLU  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 44  | CYS  | 1              |
| 1   | A     | 23  | CYS  | 1              |
| 1   | A     | 49  | LYS  | 1              |
| 1   | A     | 69  | TYR  | 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 77% for the well-defined parts and 70% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1280 |
| Number of shifts mapped to atoms        | 1280 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 0    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 130      | $0.11 \pm 0.09$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 119      | $-0.32 \pm 0.07$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 122      | $-0.03 \pm 0.05$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 122      | $-0.73 \pm 0.55$                | None needed (imprecise)    |

#### 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 77%, i.e. 877 atoms were assigned a chemical shift out of a possible 1135. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 438/449 (98%) | 177/185 (96%) | 175/178 (98%)   | 86/86 (100%)    |
| Sidechain | 397/623 (64%) | 240/400 (60%) | 157/192 (82%)   | 0/31 (0%)       |

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|          | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 42/63 (67%)    | 21/31 (68%)    | 18/27 (67%)     | 3/5 (60%)       |
| Overall  | 877/1135 (77%) | 438/616 (71%)  | 350/397 (88%)   | 89/122 (73%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 1280 atoms were assigned a chemical shift out of a possible 1826. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 622/680 (91%)   | 248/278 (89%)  | 252/272 (93%)   | 122/130 (94%)   |
| Sidechain | 600/1061 (57%)  | 343/673 (51%)  | 256/333 (77%)   | 1/55 (2%)       |
| Aromatic  | 58/85 (68%)     | 29/42 (69%)    | 25/37 (68%)     | 4/6 (67%)       |
| Overall   | 1280/1826 (70%) | 620/993 (62%)  | 533/642 (83%)   | 127/191 (66%)   |

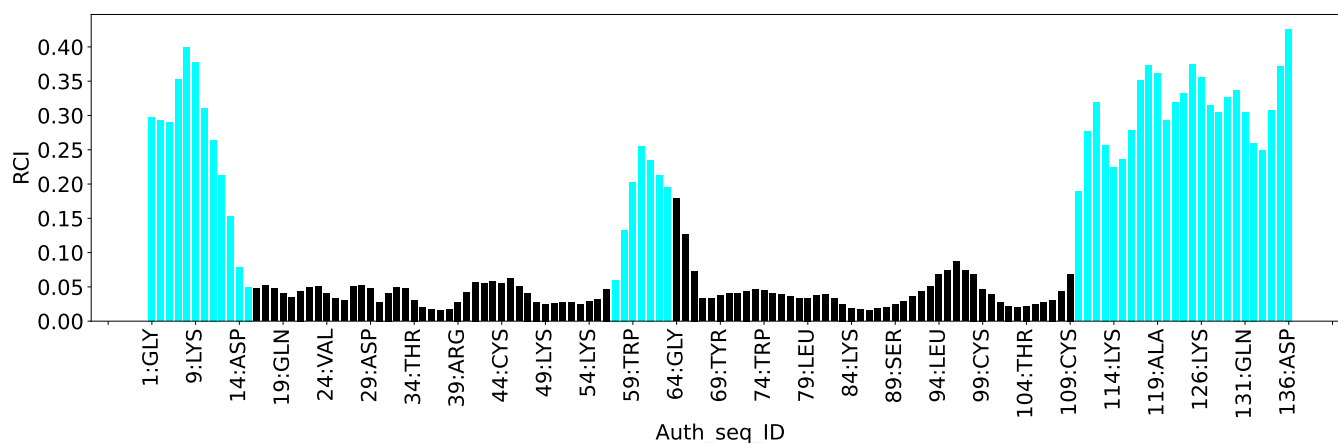
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 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                                | 833   |
| Intra-residue ( $ i-j =0$ )                              | 308   |
| Sequential ( $ i-j =1$ )                                 | 318   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 47    |
| Long range ( $ i-j \geq 5$ )                             | 160   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 125   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 7.0   |
| Number of long range restraints per residue <sup>1</sup> | 1.2   |

<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)  | 28.1                                   | 0.2     |
| 0.2-0.5 (Medium) | 33.7                                   | 0.49    |
| >0.5 (Large)     | 0.6                                    | 0.7     |



### 8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 6.3                                    | 8.21    |
| 10.0-20.0 (Medium) | 0.1                                    | 11.37   |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

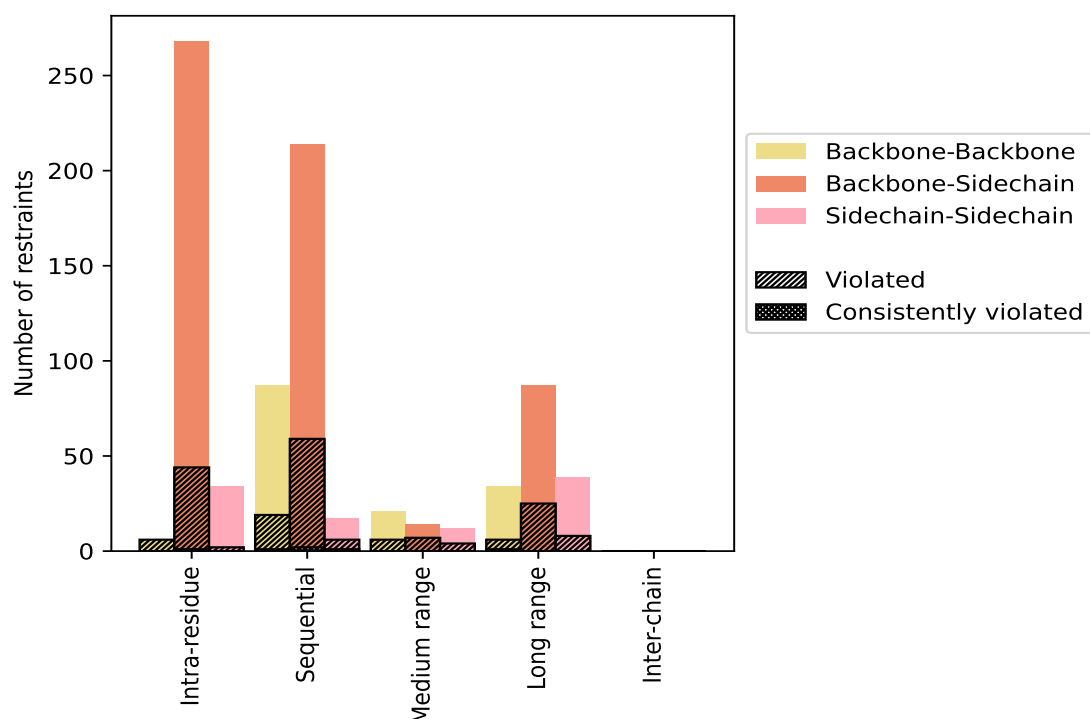
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                             | Count               | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                     |                     |
|------------------------------------------------------------|---------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|---------------------|---------------------|
|                                                            |                     |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>      | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">308</a> | <a href="#">37.0</a>  | <a href="#">52</a>    | <a href="#">16.9</a> | <a href="#">6.2</a>  | <a href="#">1</a>                  | <a href="#">0.3</a> | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 6                   | 0.7                   | 6                     | 100.0                | 0.7                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 268                 | 32.2                  | 44                    | 16.4                 | 5.3                  | 1                                  | 0.4                 | 0.1                 |
| Sidechain-Sidechain                                        | 34                  | 4.1                   | 2                     | 5.9                  | 0.2                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">318</a> | <a href="#">38.2</a>  | <a href="#">84</a>    | <a href="#">26.4</a> | <a href="#">10.1</a> | <a href="#">4</a>                  | <a href="#">1.3</a> | <a href="#">0.5</a> |
| Backbone-Backbone                                          | 87                  | 10.4                  | 19                    | 21.8                 | 2.3                  | 1                                  | 1.1                 | 0.1                 |
| Backbone-Sidechain                                         | 214                 | 25.7                  | 59                    | 27.6                 | 7.1                  | 2                                  | 0.9                 | 0.2                 |
| Sidechain-Sidechain                                        | 17                  | 2.0                   | 6                     | 35.3                 | 0.7                  | 1                                  | 5.9                 | 0.1                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">47</a>  | <a href="#">5.6</a>   | <a href="#">17</a>    | <a href="#">36.2</a> | <a href="#">2.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 21                  | 2.5                   | 6                     | 28.6                 | 0.7                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 14                  | 1.7                   | 7                     | 50.0                 | 0.8                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 12                  | 1.4                   | 4                     | 33.3                 | 0.5                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">160</a> | <a href="#">19.2</a>  | <a href="#">39</a>    | <a href="#">24.4</a> | <a href="#">4.7</a>  | <a href="#">1</a>                  | <a href="#">0.6</a> | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 34                  | 4.1                   | 6                     | 17.6                 | 0.7                  | 1                                  | 2.9                 | 0.1                 |
| Backbone-Sidechain                                         | 87                  | 10.4                  | 25                    | 28.7                 | 3.0                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 39                  | 4.7                   | 8                     | 20.5                 | 1.0                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">833</a> | <a href="#">100.0</a> | <a href="#">192</a>   | <a href="#">23.0</a> | <a href="#">23.0</a> | <a href="#">6</a>                  | <a href="#">0.7</a> | <a href="#">0.7</a> |
| Backbone-Backbone                                          | 148                 | 17.8                  | 37                    | 25.0                 | 4.4                  | 2                                  | 1.4                 | 0.2                 |
| Backbone-Sidechain                                         | 583                 | 70.0                  | 135                   | 23.2                 | 16.2                 | 3                                  | 0.5                 | 0.4                 |
| Sidechain-Sidechain                                        | 102                 | 12.2                  | 20                    | 19.6                 | 2.4                  | 1                                  | 1.0                 | 0.1                 |

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

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



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

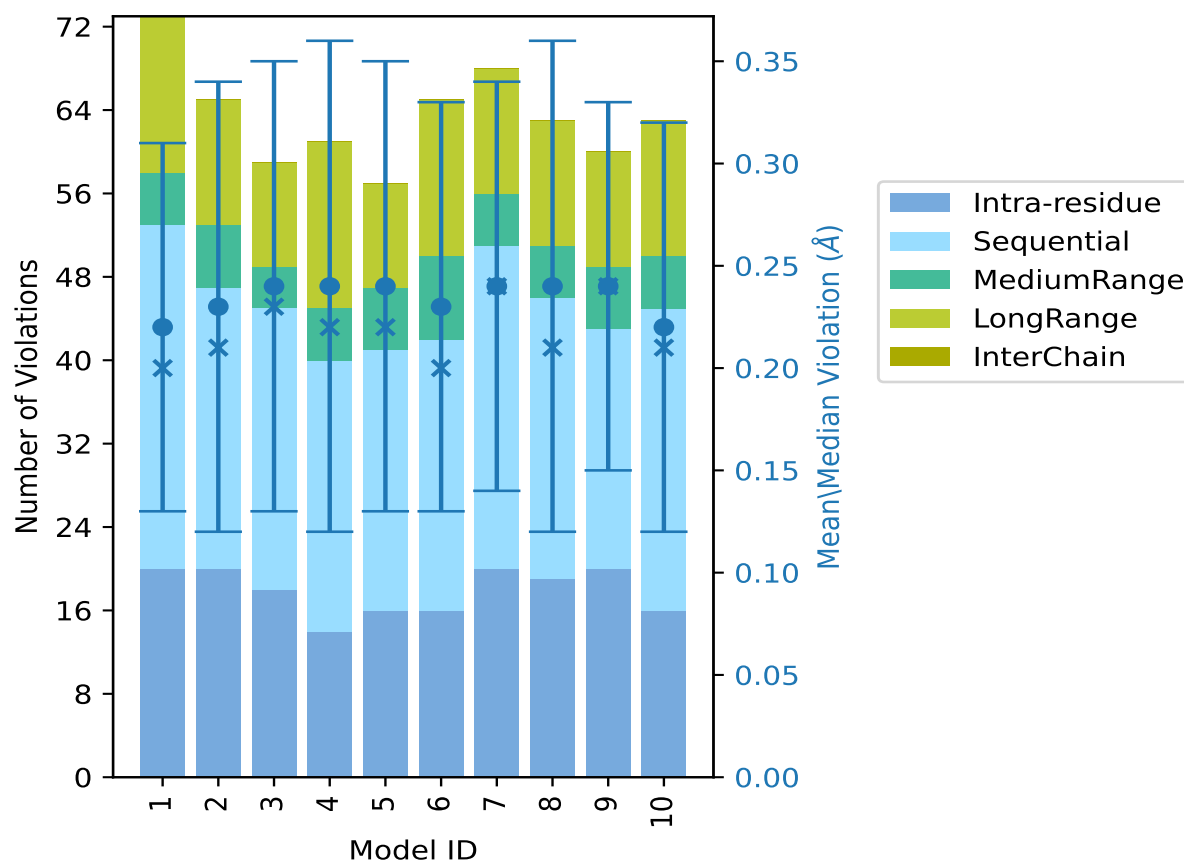
## 9.2 Distance violation statistics for each model [i](#)

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 20                   | 33              | 5               | 15              | 0               | 73    | 0.22     | 0.41    | 0.09                | 0.2        |
| 2        | 20                   | 27              | 6               | 12              | 0               | 65    | 0.23     | 0.49    | 0.11                | 0.21       |
| 3        | 18                   | 27              | 4               | 10              | 0               | 59    | 0.24     | 0.7     | 0.11                | 0.23       |
| 4        | 14                   | 26              | 5               | 16              | 0               | 61    | 0.24     | 0.68    | 0.12                | 0.22       |
| 5        | 16                   | 25              | 6               | 10              | 0               | 57    | 0.24     | 0.66    | 0.11                | 0.22       |
| 6        | 16                   | 26              | 8               | 15              | 0               | 65    | 0.23     | 0.68    | 0.1                 | 0.2        |
| 7        | 20                   | 31              | 5               | 12              | 0               | 68    | 0.24     | 0.48    | 0.1                 | 0.24       |
| 8        | 19                   | 27              | 5               | 12              | 0               | 63    | 0.24     | 0.68    | 0.12                | 0.21       |
| 9        | 20                   | 23              | 6               | 11              | 0               | 60    | 0.24     | 0.47    | 0.09                | 0.24       |
| 10       | 16                   | 29              | 5               | 13              | 0               | 63    | 0.22     | 0.58    | 0.1                 | 0.21       |

<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, 641(IR:256, SQ:234, MR:30, LR:121, 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>       | %    |
| 20                            | 33              | 6               | 15              | 0               | 74    | 1                        | 10.0 |
| 8                             | 13              | 1               | 6               | 0               | 28    | 2                        | 20.0 |
| 5                             | 11              | 6               | 5               | 0               | 27    | 3                        | 30.0 |

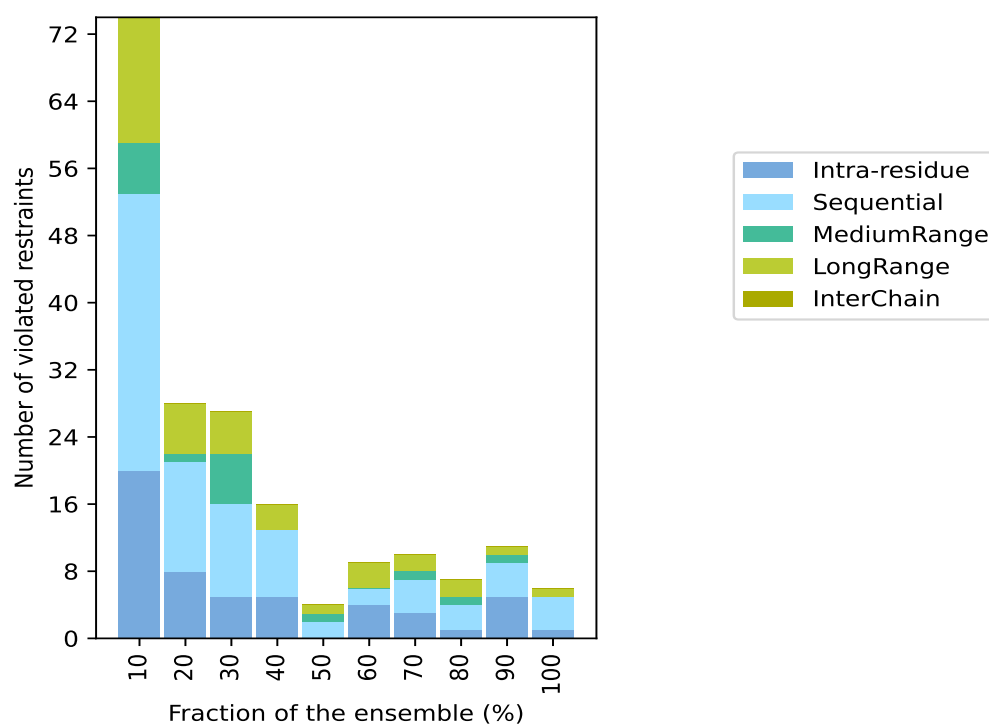
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| 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>       | %     |
| 5                             | 8               | 0               | 3               | 0               | 16    | 4                        | 40.0  |
| 0                             | 2               | 1               | 1               | 0               | 4     | 5                        | 50.0  |
| 4                             | 2               | 0               | 3               | 0               | 9     | 6                        | 60.0  |
| 3                             | 4               | 1               | 2               | 0               | 10    | 7                        | 70.0  |
| 1                             | 3               | 1               | 2               | 0               | 7     | 8                        | 80.0  |
| 5                             | 4               | 1               | 1               | 0               | 11    | 9                        | 90.0  |
| 1                             | 4               | 0               | 1               | 0               | 6     | 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 ⓘ

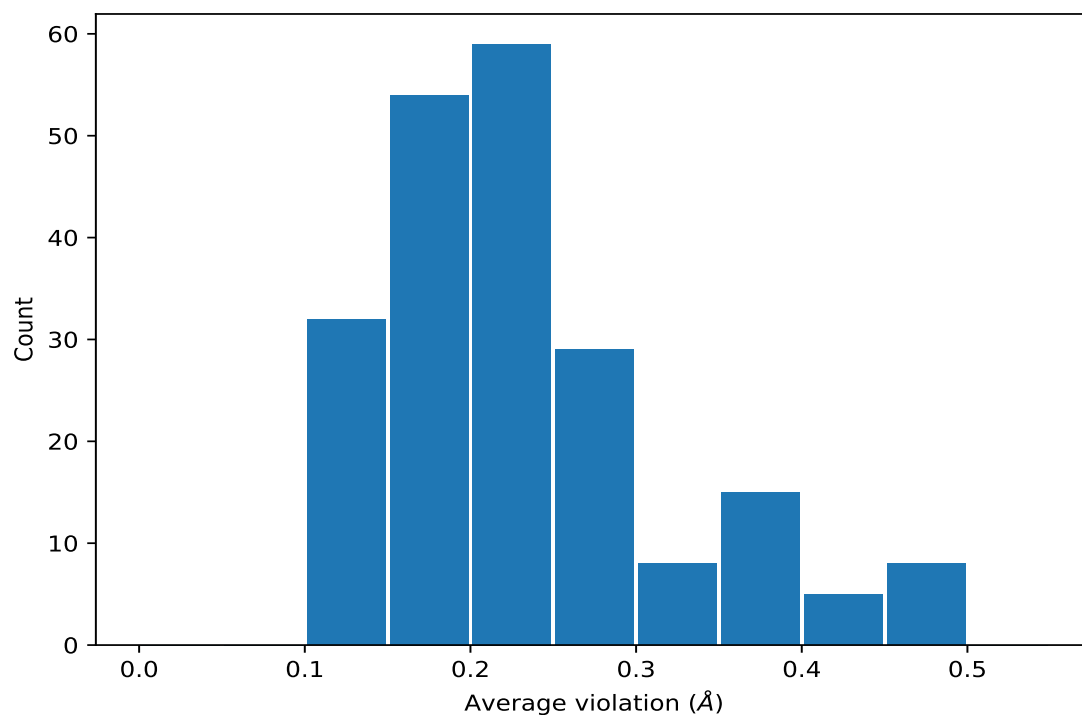


## 9.4 Most violated distance restraints in the ensemble ⓘ

### 9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,290) | 1:90:A:LEU:H   | 1:101:A:LYS:H  | 10                  | 0.41     | 0.06                | 0.43       |
| (1,581) | 1:17:A:GLU:HB2 | 1:18:A:TRP:HB3 | 10                  | 0.4      | 0.04                | 0.4        |
| (1,581) | 1:17:A:GLU:HB3 | 1:18:A:TRP:HB3 | 10                  | 0.4      | 0.04                | 0.4        |
| (1,48)  | 1:18:A:TRP:H   | 1:18:A:TRP:HE1 | 10                  | 0.31     | 0.08                | 0.32       |
| (1,25)  | 1:10:A:VAL:HB  | 1:11:A:LYS:H   | 10                  | 0.28     | 0.02                | 0.29       |
| (1,148) | 1:62:A:GLN:H   | 1:63:A:PHE:HA  | 10                  | 0.26     | 0.06                | 0.26       |
| (1,296) | 1:103:A:VAL:HA | 1:104:A:THR:HB | 10                  | 0.2      | 0.02                | 0.19       |
| (1,104) | 1:6:A:PRO:HA   | 1:7:A:GLU:H    | 9                   | 0.49     | 0.17                | 0.39       |
| (1,62)  | 1:130:A:LYS:H  | 1:130:A:LYS:HA | 9                   | 0.37     | 0.03                | 0.37       |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG2 | 9                   | 0.36     | 0.07                | 0.38       |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG3 | 9                   | 0.36     | 0.07                | 0.38       |
| (1,297) | 1:26:A:THR:HB  | 1:32:A:LEU:HA  | 9                   | 0.3      | 0.09                | 0.29       |
| (1,287) | 1:79:A:LEU:HB3 | 1:81:A:THR:H   | 9                   | 0.27     | 0.06                | 0.28       |
| (1,17)  | 1:90:A:LEU:H   | 1:90:A:LEU:HG  | 9                   | 0.25     | 0.05                | 0.26       |
| (1,291) | 1:85:A:THR:HB  | 1:86:A:ARG:H   | 9                   | 0.24     | 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) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,440) | 1:20:A:TRP:HB3  | 1:20:A:TRP:HD1  | 9                   | 0.22     | 0.02                | 0.22       |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD2  | 9                   | 0.21     | 0.09                | 0.16       |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD3  | 9                   | 0.21     | 0.09                | 0.16       |
| (1,283) | 1:81:A:THR:H    | 1:82:A:ALA:HA   | 9                   | 0.19     | 0.06                | 0.19       |
| (1,55)  | 1:18:A:TRP:H    | 1:18:A:TRP:HE3  | 9                   | 0.18     | 0.05                | 0.16       |
| (1,288) | 1:79:A:LEU:HG   | 1:81:A:THR:H    | 8                   | 0.38     | 0.05                | 0.38       |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG2 | 8                   | 0.28     | 0.06                | 0.28       |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG3 | 8                   | 0.28     | 0.06                | 0.28       |
| (1,87)  | 1:82:A:ALA:H    | 1:83:A:LEU:HG   | 8                   | 0.25     | 0.07                | 0.26       |
| (1,366) | 1:83:A:LEU:HD11 | 1:109:A:CYS:H   | 8                   | 0.21     | 0.07                | 0.22       |
| (1,366) | 1:83:A:LEU:HD12 | 1:109:A:CYS:H   | 8                   | 0.21     | 0.07                | 0.22       |
| (1,366) | 1:83:A:LEU:HD13 | 1:109:A:CYS:H   | 8                   | 0.21     | 0.07                | 0.22       |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG21 | 8                   | 0.21     | 0.05                | 0.22       |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG22 | 8                   | 0.21     | 0.05                | 0.22       |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG23 | 8                   | 0.21     | 0.05                | 0.22       |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG2  | 8                   | 0.18     | 0.03                | 0.18       |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG3  | 8                   | 0.18     | 0.03                | 0.18       |
| (1,316) | 1:89:A:SER:HA   | 1:90:A:LEU:HB3  | 8                   | 0.17     | 0.05                | 0.18       |
| (1,453) | 1:69:A:TYR:HE1  | 1:90:A:LEU:HD11 | 7                   | 0.46     | 0.06                | 0.46       |
| (1,453) | 1:69:A:TYR:HE1  | 1:90:A:LEU:HD12 | 7                   | 0.46     | 0.06                | 0.46       |
| (1,453) | 1:69:A:TYR:HE1  | 1:90:A:LEU:HD13 | 7                   | 0.46     | 0.06                | 0.46       |
| (1,453) | 1:69:A:TYR:HE2  | 1:90:A:LEU:HD11 | 7                   | 0.46     | 0.06                | 0.46       |
| (1,453) | 1:69:A:TYR:HE2  | 1:90:A:LEU:HD12 | 7                   | 0.46     | 0.06                | 0.46       |
| (1,453) | 1:69:A:TYR:HE2  | 1:90:A:LEU:HD13 | 7                   | 0.46     | 0.06                | 0.46       |
| (1,63)  | 1:9:A:LYS:H     | 1:9:A:LYS:HA    | 7                   | 0.34     | 0.05                | 0.34       |
| (1,121) | 1:72:A:GLN:HG2  | 1:73:A:ALA:H    | 7                   | 0.27     | 0.06                | 0.26       |
| (1,449) | 1:69:A:TYR:HA   | 1:69:A:TYR:HE1  | 7                   | 0.24     | 0.1                 | 0.23       |
| (1,449) | 1:69:A:TYR:HA   | 1:69:A:TYR:HE2  | 7                   | 0.24     | 0.1                 | 0.23       |
| (1,667) | 1:52:A:ARG:HD2  | 1:53:A:CYS:H    | 7                   | 0.22     | 0.06                | 0.22       |
| (1,667) | 1:52:A:ARG:HD3  | 1:53:A:CYS:H    | 7                   | 0.22     | 0.06                | 0.22       |
| (1,447) | 1:69:A:TYR:HE1  | 1:89:A:SER:HA   | 7                   | 0.21     | 0.07                | 0.21       |
| (1,447) | 1:69:A:TYR:HE2  | 1:89:A:SER:HA   | 7                   | 0.21     | 0.07                | 0.21       |
| (1,467) | 1:115:A:PRO:HB3 | 1:117:A:PRO:HD2 | 7                   | 0.21     | 0.04                | 0.22       |
| (1,330) | 1:96:A:ASN:HA   | 1:97:A:ALA:H    | 7                   | 0.21     | 0.08                | 0.17       |
| (1,36)  | 1:119:A:ALA:H   | 1:119:A:ALA:HA  | 7                   | 0.19     | 0.03                | 0.17       |
| (1,22)  | 1:78:A:ASP:HB2  | 1:79:A:LEU:H    | 7                   | 0.19     | 0.09                | 0.14       |
| (1,434) | 1:69:A:TYR:HD1  | 1:90:A:LEU:HD11 | 6                   | 0.37     | 0.08                | 0.34       |
| (1,434) | 1:69:A:TYR:HD1  | 1:90:A:LEU:HD12 | 6                   | 0.37     | 0.08                | 0.34       |
| (1,434) | 1:69:A:TYR:HD1  | 1:90:A:LEU:HD13 | 6                   | 0.37     | 0.08                | 0.34       |
| (1,434) | 1:69:A:TYR:HD2  | 1:90:A:LEU:HD11 | 6                   | 0.37     | 0.08                | 0.34       |
| (1,434) | 1:69:A:TYR:HD2  | 1:90:A:LEU:HD12 | 6                   | 0.37     | 0.08                | 0.34       |
| (1,434) | 1:69:A:TYR:HD2  | 1:90:A:LEU:HD13 | 6                   | 0.37     | 0.08                | 0.34       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,205) | 1:17:A:GLU:H    | 1:17:A:GLU:HB3  | 6                   | 0.26     | 0.06                | 0.26       |
| (1,234) | 1:76:A:GLU:H    | 1:76:A:GLU:HB3  | 6                   | 0.22     | 0.08                | 0.2        |
| (1,1)   | 1:78:A:ASP:H    | 1:85:A:THR:H    | 6                   | 0.22     | 0.09                | 0.2        |
| (1,112) | 1:47:A:THR:HB   | 1:48:A:MET:H    | 6                   | 0.21     | 0.06                | 0.22       |
| (1,133) | 1:90:A:LEU:HG   | 1:99:A:CYS:H    | 6                   | 0.19     | 0.1                 | 0.15       |
| (1,68)  | 1:133:A:LYS:H   | 1:133:A:LYS:HA  | 6                   | 0.19     | 0.03                | 0.2        |
| (1,109) | 1:8:A:LYS:H     | 1:8:A:LYS:HA    | 6                   | 0.17     | 0.04                | 0.17       |
| (1,195) | 1:102:A:THR:HB  | 1:103:A:VAL:H   | 6                   | 0.15     | 0.04                | 0.14       |
| (1,146) | 1:27:A:SER:HA   | 1:29:A:ASP:H    | 5                   | 0.28     | 0.1                 | 0.26       |
| (1,551) | 1:6:A:PRO:HB2   | 1:7:A:GLU:H     | 5                   | 0.21     | 0.01                | 0.22       |
| (1,551) | 1:6:A:PRO:HB3   | 1:7:A:GLU:H     | 5                   | 0.21     | 0.01                | 0.22       |
| (1,722) | 1:72:A:GLN:HB2  | 1:87:A:THR:H    | 5                   | 0.2      | 0.07                | 0.19       |
| (1,722) | 1:72:A:GLN:HB3  | 1:87:A:THR:H    | 5                   | 0.2      | 0.07                | 0.19       |
| (1,204) | 1:105:A:ILE:HB  | 1:106:A:SER:H   | 5                   | 0.16     | 0.02                | 0.17       |
| (1,560) | 1:9:A:LYS:HB2   | 1:10:A:VAL:H    | 4                   | 0.26     | 0.04                | 0.27       |
| (1,560) | 1:9:A:LYS:HB3   | 1:10:A:VAL:H    | 4                   | 0.26     | 0.04                | 0.27       |
| (1,602) | 1:26:A:THR:H    | 1:27:A:SER:HB2  | 4                   | 0.26     | 0.08                | 0.26       |
| (1,602) | 1:26:A:THR:H    | 1:27:A:SER:HB3  | 4                   | 0.26     | 0.08                | 0.26       |
| (1,312) | 1:7:A:GLU:HA    | 1:8:A:LYS:H     | 4                   | 0.24     | 0.12                | 0.2        |
| (1,807) | 1:111:A:LYS:HG2 | 1:112:A:LEU:H   | 4                   | 0.24     | 0.05                | 0.26       |
| (1,807) | 1:111:A:LYS:HG3 | 1:112:A:LEU:H   | 4                   | 0.24     | 0.05                | 0.26       |
| (1,201) | 1:78:A:ASP:HB2  | 1:83:A:LEU:H    | 4                   | 0.24     | 0.08                | 0.26       |
| (1,738) | 1:78:A:ASP:H    | 1:84:A:LYS:HG2  | 4                   | 0.23     | 0.06                | 0.23       |
| (1,738) | 1:78:A:ASP:H    | 1:84:A:LYS:HG3  | 4                   | 0.23     | 0.06                | 0.23       |
| (1,206) | 1:17:A:GLU:H    | 1:17:A:GLU:HB2  | 4                   | 0.22     | 0.0                 | 0.22       |
| (1,828) | 1:133:A:LYS:H   | 1:133:A:LYS:HB2 | 4                   | 0.22     | 0.03                | 0.22       |
| (1,828) | 1:133:A:LYS:H   | 1:133:A:LYS:HB3 | 4                   | 0.22     | 0.03                | 0.22       |
| (1,374) | 1:46:A:GLN:H    | 1:47:A:THR:HG21 | 4                   | 0.21     | 0.02                | 0.22       |
| (1,374) | 1:46:A:GLN:H    | 1:47:A:THR:HG22 | 4                   | 0.21     | 0.02                | 0.22       |
| (1,374) | 1:46:A:GLN:H    | 1:47:A:THR:HG23 | 4                   | 0.21     | 0.02                | 0.22       |
| (1,605) | 1:26:A:THR:HA   | 1:33:A:GLY:HA2  | 4                   | 0.2      | 0.04                | 0.18       |
| (1,605) | 1:26:A:THR:HA   | 1:33:A:GLY:HA3  | 4                   | 0.2      | 0.04                | 0.18       |
| (1,660) | 1:51:A:GLN:HA   | 1:52:A:ARG:HG2  | 4                   | 0.2      | 0.08                | 0.18       |
| (1,660) | 1:51:A:GLN:HA   | 1:52:A:ARG:HG3  | 4                   | 0.2      | 0.08                | 0.18       |
| (1,763) | 1:92:A:ARG:HA   | 1:92:A:ARG:HD2  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,763) | 1:92:A:ARG:HA   | 1:92:A:ARG:HD3  | 4                   | 0.19     | 0.07                | 0.18       |
| (1,307) | 1:26:A:THR:HG21 | 1:27:A:SER:HB2  | 4                   | 0.16     | 0.03                | 0.16       |
| (1,307) | 1:26:A:THR:HG22 | 1:27:A:SER:HB2  | 4                   | 0.16     | 0.03                | 0.16       |
| (1,307) | 1:26:A:THR:HG23 | 1:27:A:SER:HB2  | 4                   | 0.16     | 0.03                | 0.16       |
| (1,40)  | 1:113:A:THR:HB  | 1:114:A:LYS:H   | 4                   | 0.12     | 0.01                | 0.12       |
| (1,108) | 1:126:A:LYS:H   | 1:126:A:LYS:HA  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,172) | 1:54:A:LYS:H    | 1:54:A:LYS:HG3  | 4                   | 0.12     | 0.01                | 0.12       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,656) | 1:49:A:LYS:HA   | 1:49:A:LYS:HD2  | 3                   | 0.42     | 0.05                | 0.42       |
| (1,656) | 1:49:A:LYS:HA   | 1:49:A:LYS:HD3  | 3                   | 0.42     | 0.05                | 0.42       |
| (1,375) | 1:68:A:LYS:H    | 1:90:A:LEU:HD11 | 3                   | 0.38     | 0.23                | 0.32       |
| (1,375) | 1:68:A:LYS:H    | 1:90:A:LEU:HD12 | 3                   | 0.38     | 0.23                | 0.32       |
| (1,375) | 1:68:A:LYS:H    | 1:90:A:LEU:HD13 | 3                   | 0.38     | 0.23                | 0.32       |
| (1,266) | 1:63:A:PHE:HA   | 1:64:A:GLY:H    | 3                   | 0.34     | 0.15                | 0.39       |
| (1,686) | 1:61:A:LYS:HA   | 1:62:A:GLN:HG2  | 3                   | 0.33     | 0.05                | 0.32       |
| (1,686) | 1:61:A:LYS:HA   | 1:62:A:GLN:HG3  | 3                   | 0.33     | 0.05                | 0.32       |
| (1,271) | 1:40:A:THR:HB   | 1:41:A:GLY:H    | 3                   | 0.33     | 0.11                | 0.38       |
| (1,832) | 1:135:A:LEU:H   | 1:135:A:LEU:HB2 | 3                   | 0.26     | 0.01                | 0.27       |
| (1,832) | 1:135:A:LEU:H   | 1:135:A:LEU:HB3 | 3                   | 0.26     | 0.01                | 0.27       |
| (1,741) | 1:79:A:LEU:HB2  | 1:81:A:THR:H    | 3                   | 0.26     | 0.08                | 0.31       |
| (1,741) | 1:79:A:LEU:HB3  | 1:81:A:THR:H    | 3                   | 0.26     | 0.08                | 0.31       |
| (1,571) | 1:13:A:SER:HA   | 1:14:A:ASP:HB2  | 3                   | 0.25     | 0.14                | 0.18       |
| (1,571) | 1:13:A:SER:HA   | 1:14:A:ASP:HB3  | 3                   | 0.25     | 0.14                | 0.18       |
| (1,659) | 1:49:A:LYS:HG2  | 1:50:A:THR:H    | 3                   | 0.25     | 0.1                 | 0.18       |
| (1,659) | 1:49:A:LYS:HG3  | 1:50:A:THR:H    | 3                   | 0.25     | 0.1                 | 0.18       |
| (1,97)  | 1:26:A:THR:H    | 1:34:A:THR:H    | 3                   | 0.23     | 0.04                | 0.25       |
| (1,166) | 1:46:A:GLN:H    | 1:46:A:GLN:HG3  | 3                   | 0.23     | 0.09                | 0.17       |
| (1,252) | 1:28:A:GLY:H    | 1:30:A:CYS:H    | 3                   | 0.22     | 0.03                | 0.22       |
| (1,233) | 1:78:A:ASP:HB2  | 1:80:A:ASN:H    | 3                   | 0.2      | 0.03                | 0.2        |
| (1,250) | 1:30:A:CYS:H    | 1:55:A:ILE:HD11 | 3                   | 0.2      | 0.04                | 0.2        |
| (1,250) | 1:30:A:CYS:H    | 1:55:A:ILE:HD12 | 3                   | 0.2      | 0.04                | 0.2        |
| (1,250) | 1:30:A:CYS:H    | 1:55:A:ILE:HD13 | 3                   | 0.2      | 0.04                | 0.2        |
| (1,461) | 1:69:A:TYR:HD1  | 1:89:A:SER:HA   | 3                   | 0.19     | 0.04                | 0.21       |
| (1,461) | 1:69:A:TYR:HD2  | 1:89:A:SER:HA   | 3                   | 0.19     | 0.04                | 0.21       |
| (1,746) | 1:83:A:LEU:HD11 | 1:108:A:PRO:HB2 | 3                   | 0.19     | 0.05                | 0.22       |
| (1,746) | 1:83:A:LEU:HD11 | 1:108:A:PRO:HB3 | 3                   | 0.19     | 0.05                | 0.22       |
| (1,746) | 1:83:A:LEU:HD12 | 1:108:A:PRO:HB2 | 3                   | 0.19     | 0.05                | 0.22       |
| (1,746) | 1:83:A:LEU:HD12 | 1:108:A:PRO:HB3 | 3                   | 0.19     | 0.05                | 0.22       |
| (1,746) | 1:83:A:LEU:HD13 | 1:108:A:PRO:HB2 | 3                   | 0.19     | 0.05                | 0.22       |
| (1,746) | 1:83:A:LEU:HD13 | 1:108:A:PRO:HB3 | 3                   | 0.19     | 0.05                | 0.22       |
| (1,574) | 1:15:A:CYS:H    | 1:15:A:CYS:HB2  | 3                   | 0.17     | 0.04                | 0.16       |
| (1,574) | 1:15:A:CYS:H    | 1:15:A:CYS:HB3  | 3                   | 0.17     | 0.04                | 0.16       |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD11 | 3                   | 0.16     | 0.05                | 0.13       |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD12 | 3                   | 0.16     | 0.05                | 0.13       |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD13 | 3                   | 0.16     | 0.05                | 0.13       |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD21 | 3                   | 0.16     | 0.05                | 0.13       |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD22 | 3                   | 0.16     | 0.05                | 0.13       |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD23 | 3                   | 0.16     | 0.05                | 0.13       |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD11 | 3                   | 0.16     | 0.05                | 0.13       |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD12 | 3                   | 0.16     | 0.05                | 0.13       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD13 | 3                   | 0.16     | 0.05                | 0.13       |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD21 | 3                   | 0.16     | 0.05                | 0.13       |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD22 | 3                   | 0.16     | 0.05                | 0.13       |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD23 | 3                   | 0.16     | 0.05                | 0.13       |
| (1,589) | 1:19:A:GLN:HG2  | 1:20:A:TRP:H    | 3                   | 0.16     | 0.02                | 0.16       |
| (1,589) | 1:19:A:GLN:HG3  | 1:20:A:TRP:H    | 3                   | 0.16     | 0.02                | 0.16       |
| (1,292) | 1:50:A:THR:HB   | 1:51:A:GLN:H    | 3                   | 0.15     | 0.01                | 0.15       |
| (1,85)  | 1:85:A:THR:HG21 | 1:86:A:ARG:H    | 3                   | 0.14     | 0.02                | 0.15       |
| (1,85)  | 1:85:A:THR:HG22 | 1:86:A:ARG:H    | 3                   | 0.14     | 0.02                | 0.15       |
| (1,85)  | 1:85:A:THR:HG23 | 1:86:A:ARG:H    | 3                   | 0.14     | 0.02                | 0.15       |
| (1,167) | 1:97:A:ALA:HB1  | 1:98:A:GLU:H    | 3                   | 0.14     | 0.02                | 0.13       |
| (1,167) | 1:97:A:ALA:HB2  | 1:98:A:GLU:H    | 3                   | 0.14     | 0.02                | 0.13       |
| (1,167) | 1:97:A:ALA:HB3  | 1:98:A:GLU:H    | 3                   | 0.14     | 0.02                | 0.13       |
| (1,468) | 1:115:A:PRO:HB3 | 1:117:A:PRO:HD3 | 3                   | 0.14     | 0.02                | 0.14       |
| (1,70)  | 1:104:A:THR:HB  | 1:105:A:ILE:H   | 3                   | 0.13     | 0.02                | 0.14       |
| (1,231) | 1:80:A:ASN:H    | 1:80:A:ASN:HB3  | 3                   | 0.13     | 0.01                | 0.14       |
| (1,810) | 1:113:A:THR:HA  | 1:115:A:PRO:HD2 | 3                   | 0.13     | 0.01                | 0.14       |
| (1,810) | 1:113:A:THR:HA  | 1:115:A:PRO:HD3 | 3                   | 0.13     | 0.01                | 0.14       |
| (1,254) | 1:15:A:CYS:HA   | 1:16:A:GLY:H    | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,125) | 1:72:A:GLN:H    | 1:72:A:GLN:HG3  | 2                   | 0.45     | 0.01                | 0.45       |
| (1,569) | 1:12:A:LYS:H    | 1:12:A:LYS:HG2  | 2                   | 0.38     | 0.07                | 0.38       |
| (1,569) | 1:12:A:LYS:H    | 1:12:A:LYS:HG3  | 2                   | 0.38     | 0.07                | 0.38       |
| (1,28)  | 1:54:A:LYS:HG3  | 1:55:A:ILE:H    | 2                   | 0.33     | 0.04                | 0.33       |
| (1,348) | 1:94:A:LEU:HG   | 1:95:A:HIS:H    | 2                   | 0.32     | 0.1                 | 0.32       |
| (1,720) | 1:72:A:GLN:H    | 1:72:A:GLN:HG2  | 2                   | 0.3      | 0.07                | 0.3        |
| (1,720) | 1:72:A:GLN:H    | 1:72:A:GLN:HG3  | 2                   | 0.3      | 0.07                | 0.3        |
| (1,619) | 1:31:A:GLY:HA2  | 1:55:A:ILE:HG12 | 2                   | 0.26     | 0.03                | 0.26       |
| (1,619) | 1:31:A:GLY:HA2  | 1:55:A:ILE:HG13 | 2                   | 0.26     | 0.03                | 0.26       |
| (1,619) | 1:31:A:GLY:HA3  | 1:55:A:ILE:HG12 | 2                   | 0.26     | 0.03                | 0.26       |
| (1,619) | 1:31:A:GLY:HA3  | 1:55:A:ILE:HG13 | 2                   | 0.26     | 0.03                | 0.26       |
| (1,263) | 1:16:A:GLY:H    | 1:40:A:THR:H    | 2                   | 0.24     | 0.12                | 0.24       |
| (1,734) | 1:76:A:GLU:H    | 1:76:A:GLU:HG2  | 2                   | 0.24     | 0.02                | 0.24       |
| (1,734) | 1:76:A:GLU:H    | 1:76:A:GLU:HG3  | 2                   | 0.24     | 0.02                | 0.24       |
| (1,833) | 1:135:A:LEU:HB2 | 1:136:A:ASP:H   | 2                   | 0.22     | 0.04                | 0.22       |
| (1,833) | 1:135:A:LEU:HB3 | 1:136:A:ASP:H   | 2                   | 0.22     | 0.04                | 0.22       |
| (1,629) | 1:38:A:THR:HB   | 1:48:A:MET:HG2  | 2                   | 0.21     | 0.05                | 0.21       |
| (1,629) | 1:38:A:THR:HB   | 1:48:A:MET:HG3  | 2                   | 0.21     | 0.05                | 0.21       |
| (1,237) | 1:76:A:GLU:H    | 1:76:A:GLU:HB2  | 2                   | 0.2      | 0.08                | 0.2        |
| (1,688) | 1:61:A:LYS:HG2  | 1:62:A:GLN:H    | 2                   | 0.2      | 0.08                | 0.2        |
| (1,688) | 1:61:A:LYS:HG3  | 1:62:A:GLN:H    | 2                   | 0.2      | 0.08                | 0.2        |
| (1,808) | 1:112:A:LEU:H   | 1:112:A:LEU:HB2 | 2                   | 0.18     | 0.02                | 0.18       |
| (1,808) | 1:112:A:LEU:H   | 1:112:A:LEU:HB3 | 2                   | 0.18     | 0.02                | 0.18       |

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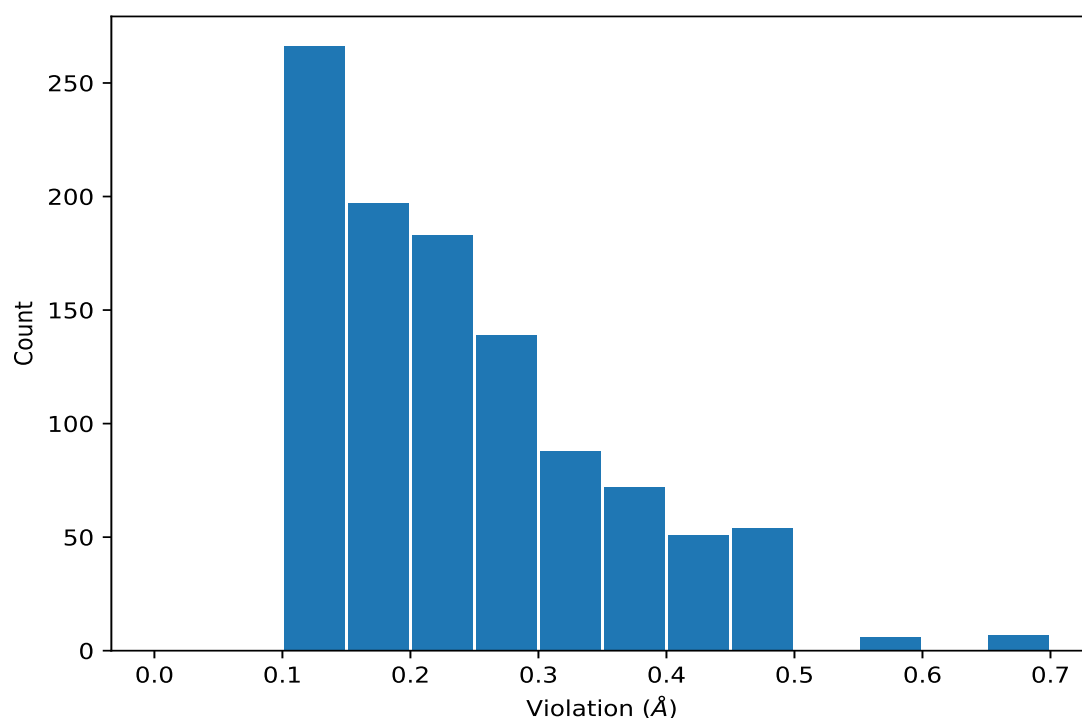
| Key     | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,827) | 1:132:A:GLU:HB2  | 1:133:A:LYS:H   | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,827) | 1:132:A:GLU:HB3  | 1:133:A:LYS:H   | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,115) | 1:26:A:THR:H     | 1:27:A:SER:HB2  | 2                   | 0.17     | 0.06                | 0.17       |
| (1,43)  | 1:90:A:LEU:HB3   | 1:101:A:LYS:H   | 2                   | 0.17     | 0.05                | 0.17       |
| (1,152) | 1:43:A:GLU:HA    | 1:44:A:CYS:H    | 2                   | 0.16     | 0.05                | 0.16       |
| (1,276) | 1:63:A:PHE:HB2   | 1:64:A:GLY:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,608) | 1:26:A:THR:HG21  | 1:27:A:SER:HB2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,608) | 1:26:A:THR:HG21  | 1:27:A:SER:HB3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,608) | 1:26:A:THR:HG22  | 1:27:A:SER:HB2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,608) | 1:26:A:THR:HG22  | 1:27:A:SER:HB3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,608) | 1:26:A:THR:HG23  | 1:27:A:SER:HB2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,608) | 1:26:A:THR:HG23  | 1:27:A:SER:HB3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,531) | 1:30:A:CYS:H     | 1:55:A:ILE:HG21 | 2                   | 0.15     | 0.02                | 0.15       |
| (1,531) | 1:30:A:CYS:H     | 1:55:A:ILE:HG22 | 2                   | 0.15     | 0.02                | 0.15       |
| (1,531) | 1:30:A:CYS:H     | 1:55:A:ILE:HG23 | 2                   | 0.15     | 0.02                | 0.15       |
| (1,420) | 1:35:A:ARG:H     | 1:36:A:GLU:HA   | 2                   | 0.14     | 0.01                | 0.14       |
| (1,766) | 1:92:A:ARG:HG2   | 1:93:A:ALA:H    | 2                   | 0.14     | 0.03                | 0.14       |
| (1,766) | 1:92:A:ARG:HG3   | 1:93:A:ALA:H    | 2                   | 0.14     | 0.03                | 0.14       |
| (1,67)  | 1:111:A:LYS:HA   | 1:112:A:LEU:H   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,478) | 1:104:A:THR:HG21 | 1:105:A:ILE:H   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,478) | 1:104:A:THR:HG22 | 1:105:A:ILE:H   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,478) | 1:104:A:THR:HG23 | 1:105:A:ILE:H   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,708) | 1:68:A:LYS:H     | 1:68:A:LYS:HG2  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,708) | 1:68:A:LYS:H     | 1:68:A:LYS:HG3  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,286) | 1:79:A:LEU:HB2   | 1:81:A:THR:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,351) | 1:90:A:LEU:HG    | 1:101:A:LYS:HA  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,193) | 1:50:A:THR:H     | 1:50:A:THR:HB   | 2                   | 0.12     | 0.0                 | 0.12       |

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

## 9.5 All violated distance restraints ⓘ

### 9.5.1 Histogram : Distribution of distance violations ⓘ

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



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

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

| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,104) | 1:6:A:PRO:HA   | 1:7:A:GLU:H     | 3        | 0.7           |
| (1,375) | 1:68:A:LYS:H   | 1:90:A:LEU:HD11 | 6        | 0.68          |
| (1,375) | 1:68:A:LYS:H   | 1:90:A:LEU:HD12 | 6        | 0.68          |
| (1,375) | 1:68:A:LYS:H   | 1:90:A:LEU:HD13 | 6        | 0.68          |
| (1,104) | 1:6:A:PRO:HA   | 1:7:A:GLU:H     | 4        | 0.68          |
| (1,104) | 1:6:A:PRO:HA   | 1:7:A:GLU:H     | 8        | 0.68          |
| (1,104) | 1:6:A:PRO:HA   | 1:7:A:GLU:H     | 5        | 0.66          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD11 | 10       | 0.58          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD12 | 10       | 0.58          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD13 | 10       | 0.58          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD11 | 10       | 0.58          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD12 | 10       | 0.58          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD13 | 10       | 0.58          |
| (1,656) | 1:49:A:LYS:HA  | 1:49:A:LYS:HD2  | 5        | 0.49          |
| (1,656) | 1:49:A:LYS:HA  | 1:49:A:LYS:HD3  | 5        | 0.49          |
| (1,434) | 1:69:A:TYR:HD1 | 1:90:A:LEU:HD11 | 2        | 0.49          |

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| Key     | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|---------|----------------|------------------|----------|---------------|
| (1,434) | 1:69:A:TYR:HD1 | 1:90:A:LEU:HD12  | 2        | 0.49          |
| (1,434) | 1:69:A:TYR:HD1 | 1:90:A:LEU:HD13  | 2        | 0.49          |
| (1,434) | 1:69:A:TYR:HD2 | 1:90:A:LEU:HD11  | 2        | 0.49          |
| (1,434) | 1:69:A:TYR:HD2 | 1:90:A:LEU:HD12  | 2        | 0.49          |
| (1,434) | 1:69:A:TYR:HD2 | 1:90:A:LEU:HD13  | 2        | 0.49          |
| (1,266) | 1:63:A:PHE:HA  | 1:64:A:GLY:H     | 2        | 0.49          |
| (1,581) | 1:17:A:GLU:HB2 | 1:18:A:TRP:HB3   | 7        | 0.48          |
| (1,581) | 1:17:A:GLU:HB3 | 1:18:A:TRP:HB3   | 7        | 0.48          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD11  | 3        | 0.48          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD12  | 3        | 0.48          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD13  | 3        | 0.48          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD11  | 3        | 0.48          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD12  | 3        | 0.48          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD13  | 3        | 0.48          |
| (1,290) | 1:90:A:LEU:H   | 1:101:A:LYS:H    | 10       | 0.48          |
| (1,125) | 1:72:A:GLN:H   | 1:72:A:GLN:HG3   | 9        | 0.47          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD11  | 2        | 0.46          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD12  | 2        | 0.46          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD13  | 2        | 0.46          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD11  | 2        | 0.46          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD12  | 2        | 0.46          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD13  | 2        | 0.46          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD11  | 4        | 0.46          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD12  | 4        | 0.46          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD13  | 4        | 0.46          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD11  | 4        | 0.46          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD12  | 4        | 0.46          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD13  | 4        | 0.46          |
| (1,434) | 1:69:A:TYR:HD1 | 1:90:A:LEU:HD11  | 8        | 0.46          |
| (1,434) | 1:69:A:TYR:HD1 | 1:90:A:LEU:HD12  | 8        | 0.46          |
| (1,434) | 1:69:A:TYR:HD1 | 1:90:A:LEU:HD13  | 8        | 0.46          |
| (1,434) | 1:69:A:TYR:HD2 | 1:90:A:LEU:HD11  | 8        | 0.46          |
| (1,434) | 1:69:A:TYR:HD2 | 1:90:A:LEU:HD12  | 8        | 0.46          |
| (1,434) | 1:69:A:TYR:HD2 | 1:90:A:LEU:HD13  | 8        | 0.46          |
| (1,290) | 1:90:A:LEU:H   | 1:101:A:LYS:H    | 8        | 0.46          |
| (1,581) | 1:17:A:GLU:HB2 | 1:18:A:TRP:HB3   | 4        | 0.45          |
| (1,581) | 1:17:A:GLU:HB3 | 1:18:A:TRP:HB3   | 4        | 0.45          |
| (1,569) | 1:12:A:LYS:H   | 1:12:A:LYS:HG2   | 9        | 0.45          |
| (1,569) | 1:12:A:LYS:H   | 1:12:A:LYS:HG3   | 9        | 0.45          |
| (1,525) | 1:104:A:THR:HA | 1:105:A:ILE:HG21 | 4        | 0.45          |
| (1,525) | 1:104:A:THR:HA | 1:105:A:ILE:HG22 | 4        | 0.45          |
| (1,525) | 1:104:A:THR:HA | 1:105:A:ILE:HG23 | 4        | 0.45          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD11 | 8        | 0.45          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD12 | 8        | 0.45          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD13 | 8        | 0.45          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD11 | 8        | 0.45          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD12 | 8        | 0.45          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD13 | 8        | 0.45          |
| (1,290) | 1:90:A:LEU:H   | 1:101:A:LYS:H   | 2        | 0.45          |
| (1,290) | 1:90:A:LEU:H   | 1:101:A:LYS:H   | 7        | 0.45          |
| (1,288) | 1:79:A:LEU:HG  | 1:81:A:THR:H    | 6        | 0.45          |
| (1,581) | 1:17:A:GLU:HB2 | 1:18:A:TRP:HB3  | 2        | 0.44          |
| (1,581) | 1:17:A:GLU:HB3 | 1:18:A:TRP:HB3  | 2        | 0.44          |
| (1,571) | 1:13:A:SER:HA  | 1:14:A:ASP:HB2  | 3        | 0.44          |
| (1,571) | 1:13:A:SER:HA  | 1:14:A:ASP:HB3  | 3        | 0.44          |
| (1,290) | 1:90:A:LEU:H   | 1:101:A:LYS:H   | 5        | 0.44          |
| (1,125) | 1:72:A:GLN:H   | 1:72:A:GLN:HG3  | 4        | 0.44          |
| (1,581) | 1:17:A:GLU:HB2 | 1:18:A:TRP:HB3  | 3        | 0.43          |
| (1,581) | 1:17:A:GLU:HB3 | 1:18:A:TRP:HB3  | 3        | 0.43          |
| (1,312) | 1:7:A:GLU:HA   | 1:8:A:LYS:H     | 7        | 0.43          |
| (1,288) | 1:79:A:LEU:HG  | 1:81:A:THR:H    | 5        | 0.43          |
| (1,271) | 1:40:A:THR:HB  | 1:41:A:GLY:H    | 8        | 0.43          |
| (1,247) | 1:28:A:GLY:HA2 | 1:30:A:CYS:H    | 10       | 0.43          |
| (1,62)  | 1:130:A:LYS:H  | 1:130:A:LYS:HA  | 6        | 0.43          |
| (1,48)  | 1:18:A:TRP:H   | 1:18:A:TRP:HE1  | 6        | 0.43          |
| (1,656) | 1:49:A:LYS:HA  | 1:49:A:LYS:HD2  | 7        | 0.42          |
| (1,656) | 1:49:A:LYS:HA  | 1:49:A:LYS:HD3  | 7        | 0.42          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD11 | 7        | 0.42          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD12 | 7        | 0.42          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD13 | 7        | 0.42          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD11 | 7        | 0.42          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD12 | 7        | 0.42          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD13 | 7        | 0.42          |
| (1,348) | 1:94:A:LEU:HG  | 1:95:A:HIS:H    | 7        | 0.42          |
| (1,297) | 1:26:A:THR:HB  | 1:32:A:LEU:HA   | 2        | 0.42          |
| (1,290) | 1:90:A:LEU:H   | 1:101:A:LYS:H   | 4        | 0.42          |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG2  | 4        | 0.41          |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG3  | 4        | 0.41          |
| (1,581) | 1:17:A:GLU:HB2 | 1:18:A:TRP:HB3  | 8        | 0.41          |
| (1,581) | 1:17:A:GLU:HB3 | 1:18:A:TRP:HB3  | 8        | 0.41          |
| (1,334) | 1:72:A:GLN:HA  | 1:72:A:GLN:HG3  | 10       | 0.41          |
| (1,297) | 1:26:A:THR:HB  | 1:32:A:LEU:HA   | 8        | 0.41          |
| (1,288) | 1:79:A:LEU:HG  | 1:81:A:THR:H    | 3        | 0.41          |
| (1,180) | 1:15:A:CYS:H   | 1:16:A:GLY:H    | 2        | 0.41          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,146) | 1:27:A:SER:HA  | 1:29:A:ASP:H    | 4        | 0.41          |
| (1,133) | 1:90:A:LEU:HG  | 1:99:A:CYS:H    | 9        | 0.41          |
| (1,48)  | 1:18:A:TRP:H   | 1:18:A:TRP:HE1  | 4        | 0.41          |
| (1,22)  | 1:78:A:ASP:HB2 | 1:79:A:LEU:H    | 1        | 0.41          |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG2  | 1        | 0.4           |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG3  | 1        | 0.4           |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG2  | 5        | 0.4           |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG3  | 5        | 0.4           |
| (1,686) | 1:61:A:LYS:HA  | 1:62:A:GLN:HG2  | 5        | 0.4           |
| (1,686) | 1:61:A:LYS:HA  | 1:62:A:GLN:HG3  | 5        | 0.4           |
| (1,449) | 1:69:A:TYR:HA  | 1:69:A:TYR:HE1  | 8        | 0.4           |
| (1,449) | 1:69:A:TYR:HA  | 1:69:A:TYR:HE2  | 8        | 0.4           |
| (1,290) | 1:90:A:LEU:H   | 1:101:A:LYS:H   | 3        | 0.4           |
| (1,288) | 1:79:A:LEU:HG  | 1:81:A:THR:H    | 1        | 0.4           |
| (1,121) | 1:72:A:GLN:HG2 | 1:73:A:ALA:H    | 8        | 0.4           |
| (1,64)  | 1:133:A:LYS:HA | 1:134:A:MET:H   | 1        | 0.4           |
| (1,63)  | 1:9:A:LYS:H    | 1:9:A:LYS:HA    | 3        | 0.4           |
| (1,63)  | 1:9:A:LYS:H    | 1:9:A:LYS:HA    | 9        | 0.4           |
| (1,754) | 1:90:A:LEU:HB3 | 1:100:A:GLN:HG2 | 7        | 0.39          |
| (1,754) | 1:90:A:LEU:HB3 | 1:100:A:GLN:HG3 | 7        | 0.39          |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG2  | 7        | 0.39          |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG3  | 7        | 0.39          |
| (1,659) | 1:49:A:LYS:HG2 | 1:50:A:THR:H    | 9        | 0.39          |
| (1,659) | 1:49:A:LYS:HG3 | 1:50:A:THR:H    | 9        | 0.39          |
| (1,266) | 1:63:A:PHE:HA  | 1:64:A:GLY:H    | 6        | 0.39          |
| (1,104) | 1:6:A:PRO:HA   | 1:7:A:GLU:H     | 1        | 0.39          |
| (1,104) | 1:6:A:PRO:HA   | 1:7:A:GLU:H     | 10       | 0.39          |
| (1,1)   | 1:78:A:ASP:H   | 1:85:A:THR:H    | 1        | 0.39          |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG2  | 9        | 0.38          |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG3  | 9        | 0.38          |
| (1,602) | 1:26:A:THR:H   | 1:27:A:SER:HB2  | 6        | 0.38          |
| (1,602) | 1:26:A:THR:H   | 1:27:A:SER:HB3  | 6        | 0.38          |
| (1,581) | 1:17:A:GLU:HB2 | 1:18:A:TRP:HB3  | 10       | 0.38          |
| (1,581) | 1:17:A:GLU:HB3 | 1:18:A:TRP:HB3  | 10       | 0.38          |
| (1,502) | 1:81:A:THR:HA  | 1:81:A:THR:HG21 | 6        | 0.38          |
| (1,502) | 1:81:A:THR:HA  | 1:81:A:THR:HG22 | 6        | 0.38          |
| (1,502) | 1:81:A:THR:HA  | 1:81:A:THR:HG23 | 6        | 0.38          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD11 | 5        | 0.38          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD12 | 5        | 0.38          |
| (1,453) | 1:69:A:TYR:HE1 | 1:90:A:LEU:HD13 | 5        | 0.38          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD11 | 5        | 0.38          |
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD12 | 5        | 0.38          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,453) | 1:69:A:TYR:HE2 | 1:90:A:LEU:HD13 | 5        | 0.38          |
| (1,290) | 1:90:A:LEU:H   | 1:101:A:LYS:H   | 1        | 0.38          |
| (1,271) | 1:40:A:THR:HB  | 1:41:A:GLY:H    | 3        | 0.38          |
| (1,148) | 1:62:A:GLN:H   | 1:63:A:PHE:HA   | 8        | 0.38          |
| (1,62)  | 1:130:A:LYS:H  | 1:130:A:LYS:HA  | 8        | 0.38          |
| (1,48)  | 1:18:A:TRP:H   | 1:18:A:TRP:HE1  | 7        | 0.38          |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG2  | 8        | 0.37          |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG3  | 8        | 0.37          |
| (1,720) | 1:72:A:GLN:H   | 1:72:A:GLN:HG2  | 4        | 0.37          |
| (1,720) | 1:72:A:GLN:H   | 1:72:A:GLN:HG3  | 4        | 0.37          |
| (1,581) | 1:17:A:GLU:HB2 | 1:18:A:TRP:HB3  | 9        | 0.37          |
| (1,581) | 1:17:A:GLU:HB3 | 1:18:A:TRP:HB3  | 9        | 0.37          |
| (1,434) | 1:69:A:TYR:HD1 | 1:90:A:LEU:HD11 | 5        | 0.37          |
| (1,434) | 1:69:A:TYR:HD1 | 1:90:A:LEU:HD12 | 5        | 0.37          |
| (1,434) | 1:69:A:TYR:HD1 | 1:90:A:LEU:HD13 | 5        | 0.37          |
| (1,434) | 1:69:A:TYR:HD2 | 1:90:A:LEU:HD11 | 5        | 0.37          |
| (1,434) | 1:69:A:TYR:HD2 | 1:90:A:LEU:HD12 | 5        | 0.37          |
| (1,434) | 1:69:A:TYR:HD2 | 1:90:A:LEU:HD13 | 5        | 0.37          |
| (1,297) | 1:26:A:THR:HB  | 1:32:A:LEU:HA   | 4        | 0.37          |
| (1,288) | 1:79:A:LEU:HG  | 1:81:A:THR:H    | 8        | 0.37          |
| (1,287) | 1:79:A:LEU:HB3 | 1:81:A:THR:H    | 6        | 0.37          |
| (1,234) | 1:76:A:GLU:H   | 1:76:A:GLU:HB3  | 9        | 0.37          |
| (1,63)  | 1:9:A:LYS:H    | 1:9:A:LYS:HA    | 10       | 0.37          |
| (1,62)  | 1:130:A:LYS:H  | 1:130:A:LYS:HA  | 2        | 0.37          |
| (1,62)  | 1:130:A:LYS:H  | 1:130:A:LYS:HA  | 4        | 0.37          |
| (1,62)  | 1:130:A:LYS:H  | 1:130:A:LYS:HA  | 9        | 0.37          |
| (1,28)  | 1:54:A:LYS:HG3 | 1:55:A:ILE:H    | 3        | 0.37          |
| (1,819) | 1:126:A:LYS:H  | 1:126:A:LYS:HG2 | 7        | 0.36          |
| (1,819) | 1:126:A:LYS:H  | 1:126:A:LYS:HG3 | 7        | 0.36          |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG2  | 10       | 0.36          |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG3  | 10       | 0.36          |
| (1,656) | 1:49:A:LYS:HA  | 1:49:A:LYS:HD2  | 1        | 0.36          |
| (1,656) | 1:49:A:LYS:HA  | 1:49:A:LYS:HD3  | 1        | 0.36          |
| (1,581) | 1:17:A:GLU:HB2 | 1:18:A:TRP:HB3  | 1        | 0.36          |
| (1,581) | 1:17:A:GLU:HB3 | 1:18:A:TRP:HB3  | 1        | 0.36          |
| (1,581) | 1:17:A:GLU:HB2 | 1:18:A:TRP:HB3  | 6        | 0.36          |
| (1,581) | 1:17:A:GLU:HB3 | 1:18:A:TRP:HB3  | 6        | 0.36          |
| (1,263) | 1:16:A:GLY:H   | 1:40:A:THR:H    | 2        | 0.36          |
| (1,146) | 1:27:A:SER:HA  | 1:29:A:ASP:H    | 8        | 0.36          |
| (1,62)  | 1:130:A:LYS:H  | 1:130:A:LYS:HA  | 1        | 0.36          |
| (1,62)  | 1:130:A:LYS:H  | 1:130:A:LYS:HA  | 5        | 0.36          |
| (1,48)  | 1:18:A:TRP:H   | 1:18:A:TRP:HE1  | 8        | 0.36          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD2  | 4        | 0.35          |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD3  | 4        | 0.35          |
| (1,581) | 1:17:A:GLU:HB2  | 1:18:A:TRP:HB3  | 5        | 0.35          |
| (1,581) | 1:17:A:GLU:HB3  | 1:18:A:TRP:HB3  | 5        | 0.35          |
| (1,297) | 1:26:A:THR:HB   | 1:32:A:LEU:HA   | 6        | 0.35          |
| (1,166) | 1:46:A:GLN:H    | 1:46:A:GLN:HG3  | 7        | 0.35          |
| (1,642) | 1:45:A:LYS:HA   | 1:45:A:LYS:HD2  | 2        | 0.34          |
| (1,642) | 1:45:A:LYS:HA   | 1:45:A:LYS:HD3  | 2        | 0.34          |
| (1,330) | 1:96:A:ASN:HA   | 1:97:A:ALA:H    | 1        | 0.34          |
| (1,290) | 1:90:A:LEU:H    | 1:101:A:LYS:H   | 9        | 0.34          |
| (1,63)  | 1:9:A:LYS:H     | 1:9:A:LYS:HA    | 8        | 0.34          |
| (1,62)  | 1:130:A:LYS:H   | 1:130:A:LYS:HA  | 3        | 0.34          |
| (1,62)  | 1:130:A:LYS:H   | 1:130:A:LYS:HA  | 7        | 0.34          |
| (1,812) | 1:115:A:PRO:HB3 | 1:117:A:PRO:HD2 | 8        | 0.33          |
| (1,812) | 1:115:A:PRO:HB3 | 1:117:A:PRO:HD3 | 8        | 0.33          |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD2  | 3        | 0.33          |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD3  | 3        | 0.33          |
| (1,660) | 1:51:A:GLN:HA   | 1:52:A:ARG:HG2  | 7        | 0.33          |
| (1,660) | 1:51:A:GLN:HA   | 1:52:A:ARG:HG3  | 7        | 0.33          |
| (1,447) | 1:69:A:TYR:HE1  | 1:89:A:SER:HA   | 5        | 0.33          |
| (1,447) | 1:69:A:TYR:HE2  | 1:89:A:SER:HA   | 5        | 0.33          |
| (1,291) | 1:85:A:THR:HB   | 1:86:A:ARG:H    | 1        | 0.33          |
| (1,288) | 1:79:A:LEU:HG   | 1:81:A:THR:H    | 4        | 0.33          |
| (1,205) | 1:17:A:GLU:H    | 1:17:A:GLU:HB3  | 7        | 0.33          |
| (1,121) | 1:72:A:GLN:HG2  | 1:73:A:ALA:H    | 7        | 0.33          |
| (1,104) | 1:6:A:PRO:HA    | 1:7:A:GLU:H     | 2        | 0.33          |
| (1,48)  | 1:18:A:TRP:H    | 1:18:A:TRP:HE1  | 5        | 0.33          |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG2 | 1        | 0.32          |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG3 | 1        | 0.32          |
| (1,741) | 1:79:A:LEU:HB2  | 1:81:A:THR:H    | 2        | 0.32          |
| (1,741) | 1:79:A:LEU:HB3  | 1:81:A:THR:H    | 2        | 0.32          |
| (1,686) | 1:61:A:LYS:HA   | 1:62:A:GLN:HG2  | 7        | 0.32          |
| (1,686) | 1:61:A:LYS:HA   | 1:62:A:GLN:HG3  | 7        | 0.32          |
| (1,667) | 1:52:A:ARG:HD2  | 1:53:A:CYS:H    | 3        | 0.32          |
| (1,667) | 1:52:A:ARG:HD3  | 1:53:A:CYS:H    | 3        | 0.32          |
| (1,560) | 1:9:A:LYS:HB2   | 1:10:A:VAL:H    | 6        | 0.32          |
| (1,560) | 1:9:A:LYS:HB3   | 1:10:A:VAL:H    | 6        | 0.32          |
| (1,449) | 1:69:A:TYR:HA   | 1:69:A:TYR:HE1  | 2        | 0.32          |
| (1,449) | 1:69:A:TYR:HA   | 1:69:A:TYR:HE2  | 2        | 0.32          |
| (1,449) | 1:69:A:TYR:HA   | 1:69:A:TYR:HE1  | 6        | 0.32          |
| (1,449) | 1:69:A:TYR:HA   | 1:69:A:TYR:HE2  | 6        | 0.32          |
| (1,375) | 1:68:A:LYS:H    | 1:90:A:LEU:HD11 | 9        | 0.32          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,375) | 1:68:A:LYS:H    | 1:90:A:LEU:HD12 | 9        | 0.32          |
| (1,375) | 1:68:A:LYS:H    | 1:90:A:LEU:HD13 | 9        | 0.32          |
| (1,366) | 1:83:A:LEU:HD11 | 1:109:A:CYS:H   | 9        | 0.32          |
| (1,366) | 1:83:A:LEU:HD12 | 1:109:A:CYS:H   | 9        | 0.32          |
| (1,366) | 1:83:A:LEU:HD13 | 1:109:A:CYS:H   | 9        | 0.32          |
| (1,288) | 1:79:A:LEU:HG   | 1:81:A:THR:H    | 7        | 0.32          |
| (1,104) | 1:6:A:PRO:HA    | 1:7:A:GLU:H     | 6        | 0.32          |
| (1,87)  | 1:82:A:ALA:H    | 1:83:A:LEU:HG   | 2        | 0.32          |
| (1,87)  | 1:82:A:ALA:H    | 1:83:A:LEU:HG   | 4        | 0.32          |
| (1,63)  | 1:9:A:LYS:H     | 1:9:A:LYS:HA    | 1        | 0.32          |
| (1,27)  | 1:54:A:LYS:HG2  | 1:55:A:ILE:H    | 2        | 0.32          |
| (1,17)  | 1:90:A:LEU:H    | 1:90:A:LEU:HG   | 8        | 0.32          |
| (1,745) | 1:83:A:LEU:HA   | 1:84:A:LYS:HG2  | 6        | 0.31          |
| (1,745) | 1:83:A:LEU:HA   | 1:84:A:LYS:HG3  | 6        | 0.31          |
| (1,741) | 1:79:A:LEU:HB2  | 1:81:A:THR:H    | 9        | 0.31          |
| (1,741) | 1:79:A:LEU:HB3  | 1:81:A:THR:H    | 9        | 0.31          |
| (1,738) | 1:78:A:ASP:H    | 1:84:A:LYS:HG2  | 2        | 0.31          |
| (1,738) | 1:78:A:ASP:H    | 1:84:A:LYS:HG3  | 2        | 0.31          |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD2  | 7        | 0.31          |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD3  | 7        | 0.31          |
| (1,569) | 1:12:A:LYS:H    | 1:12:A:LYS:HG2  | 3        | 0.31          |
| (1,569) | 1:12:A:LYS:H    | 1:12:A:LYS:HG3  | 3        | 0.31          |
| (1,434) | 1:69:A:TYR:HD1  | 1:90:A:LEU:HD11 | 4        | 0.31          |
| (1,434) | 1:69:A:TYR:HD1  | 1:90:A:LEU:HD12 | 4        | 0.31          |
| (1,434) | 1:69:A:TYR:HD1  | 1:90:A:LEU:HD13 | 4        | 0.31          |
| (1,434) | 1:69:A:TYR:HD2  | 1:90:A:LEU:HD11 | 4        | 0.31          |
| (1,434) | 1:69:A:TYR:HD2  | 1:90:A:LEU:HD12 | 4        | 0.31          |
| (1,434) | 1:69:A:TYR:HD2  | 1:90:A:LEU:HD13 | 4        | 0.31          |
| (1,434) | 1:69:A:TYR:HD1  | 1:90:A:LEU:HD11 | 7        | 0.31          |
| (1,434) | 1:69:A:TYR:HD1  | 1:90:A:LEU:HD12 | 7        | 0.31          |
| (1,434) | 1:69:A:TYR:HD1  | 1:90:A:LEU:HD13 | 7        | 0.31          |
| (1,434) | 1:69:A:TYR:HD2  | 1:90:A:LEU:HD11 | 7        | 0.31          |
| (1,434) | 1:69:A:TYR:HD2  | 1:90:A:LEU:HD12 | 7        | 0.31          |
| (1,434) | 1:69:A:TYR:HD2  | 1:90:A:LEU:HD13 | 7        | 0.31          |
| (1,291) | 1:85:A:THR:HB   | 1:86:A:ARG:H    | 9        | 0.31          |
| (1,205) | 1:17:A:GLU:H    | 1:17:A:GLU:HB3  | 2        | 0.31          |
| (1,87)  | 1:82:A:ALA:H    | 1:83:A:LEU:HG   | 6        | 0.31          |
| (1,87)  | 1:82:A:ALA:H    | 1:83:A:LEU:HG   | 10       | 0.31          |
| (1,25)  | 1:10:A:VAL:HB   | 1:11:A:LYS:H    | 10       | 0.31          |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG2 | 9        | 0.3           |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG3 | 9        | 0.3           |
| (1,447) | 1:69:A:TYR:HE1  | 1:89:A:SER:HA   | 3        | 0.3           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,447) | 1:69:A:TYR:HE2  | 1:89:A:SER:HA   | 3        | 0.3           |
| (1,330) | 1:96:A:ASN:HA   | 1:97:A:ALA:H    | 8        | 0.3           |
| (1,288) | 1:79:A:LEU:HG   | 1:81:A:THR:H    | 10       | 0.3           |
| (1,287) | 1:79:A:LEU:HB3  | 1:81:A:THR:H    | 9        | 0.3           |
| (1,201) | 1:78:A:ASP:HB2  | 1:83:A:LEU:H    | 1        | 0.3           |
| (1,148) | 1:62:A:GLN:H    | 1:63:A:PHE:HA   | 10       | 0.3           |
| (1,48)  | 1:18:A:TRP:H    | 1:18:A:TRP:HE1  | 1        | 0.3           |
| (1,25)  | 1:10:A:VAL:HB   | 1:11:A:LYS:H    | 2        | 0.3           |
| (1,25)  | 1:10:A:VAL:HB   | 1:11:A:LYS:H    | 4        | 0.3           |
| (1,25)  | 1:10:A:VAL:HB   | 1:11:A:LYS:H    | 6        | 0.3           |
| (1,807) | 1:111:A:LYS:HG2 | 1:112:A:LEU:H   | 6        | 0.29          |
| (1,807) | 1:111:A:LYS:HG3 | 1:112:A:LEU:H   | 6        | 0.29          |
| (1,722) | 1:72:A:GLN:HB2  | 1:87:A:THR:H    | 3        | 0.29          |
| (1,722) | 1:72:A:GLN:HB3  | 1:87:A:THR:H    | 3        | 0.29          |
| (1,688) | 1:61:A:LYS:HG2  | 1:62:A:GLN:H    | 9        | 0.29          |
| (1,688) | 1:61:A:LYS:HG3  | 1:62:A:GLN:H    | 9        | 0.29          |
| (1,297) | 1:26:A:THR:HB   | 1:32:A:LEU:HA   | 7        | 0.29          |
| (1,291) | 1:85:A:THR:HB   | 1:86:A:ARG:H    | 10       | 0.29          |
| (1,287) | 1:79:A:LEU:HB3  | 1:81:A:THR:H    | 7        | 0.29          |
| (1,237) | 1:76:A:GLU:H    | 1:76:A:GLU:HB2  | 2        | 0.29          |
| (1,205) | 1:17:A:GLU:H    | 1:17:A:GLU:HB3  | 4        | 0.29          |
| (1,201) | 1:78:A:ASP:HB2  | 1:83:A:LEU:H    | 4        | 0.29          |
| (1,148) | 1:62:A:GLN:H    | 1:63:A:PHE:HA   | 1        | 0.29          |
| (1,148) | 1:62:A:GLN:H    | 1:63:A:PHE:HA   | 3        | 0.29          |
| (1,28)  | 1:54:A:LYS:HG3  | 1:55:A:ILE:H    | 1        | 0.29          |
| (1,25)  | 1:10:A:VAL:HB   | 1:11:A:LYS:H    | 8        | 0.29          |
| (1,17)  | 1:90:A:LEU:H    | 1:90:A:LEU:HG   | 1        | 0.29          |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG2 | 4        | 0.28          |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG3 | 4        | 0.28          |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG2 | 5        | 0.28          |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG3 | 5        | 0.28          |
| (1,686) | 1:61:A:LYS:HA   | 1:62:A:GLN:HG2  | 4        | 0.28          |
| (1,686) | 1:61:A:LYS:HA   | 1:62:A:GLN:HG3  | 4        | 0.28          |
| (1,641) | 1:45:A:LYS:HA   | 1:45:A:LYS:HG2  | 2        | 0.28          |
| (1,641) | 1:45:A:LYS:HA   | 1:45:A:LYS:HG3  | 2        | 0.28          |
| (1,619) | 1:31:A:GLY:HA2  | 1:55:A:ILE:HG12 | 5        | 0.28          |
| (1,619) | 1:31:A:GLY:HA2  | 1:55:A:ILE:HG13 | 5        | 0.28          |
| (1,619) | 1:31:A:GLY:HA3  | 1:55:A:ILE:HG12 | 5        | 0.28          |
| (1,619) | 1:31:A:GLY:HA3  | 1:55:A:ILE:HG13 | 5        | 0.28          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG21 | 9        | 0.28          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG22 | 9        | 0.28          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG23 | 9        | 0.28          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,287) | 1:79:A:LEU:HB3  | 1:81:A:THR:H    | 2        | 0.28          |
| (1,287) | 1:79:A:LEU:HB3  | 1:81:A:THR:H    | 5        | 0.28          |
| (1,283) | 1:81:A:THR:H    | 1:82:A:ALA:HA   | 6        | 0.28          |
| (1,148) | 1:62:A:GLN:H    | 1:63:A:PHE:HA   | 6        | 0.28          |
| (1,121) | 1:72:A:GLN:HG2  | 1:73:A:ALA:H    | 6        | 0.28          |
| (1,116) | 1:60:A:LYS:HA   | 1:61:A:LYS:H    | 9        | 0.28          |
| (1,112) | 1:47:A:THR:HB   | 1:48:A:MET:H    | 9        | 0.28          |
| (1,104) | 1:6:A:PRO:HA    | 1:7:A:GLU:H     | 7        | 0.28          |
| (1,63)  | 1:9:A:LYS:H     | 1:9:A:LYS:HA    | 7        | 0.28          |
| (1,48)  | 1:18:A:TRP:H    | 1:18:A:TRP:HE1  | 3        | 0.28          |
| (1,25)  | 1:10:A:VAL:HB   | 1:11:A:LYS:H    | 1        | 0.28          |
| (1,17)  | 1:90:A:LEU:H    | 1:90:A:LEU:HG   | 9        | 0.28          |
| (1,832) | 1:135:A:LEU:H   | 1:135:A:LEU:HB2 | 4        | 0.27          |
| (1,832) | 1:135:A:LEU:H   | 1:135:A:LEU:HB3 | 4        | 0.27          |
| (1,832) | 1:135:A:LEU:H   | 1:135:A:LEU:HB2 | 10       | 0.27          |
| (1,832) | 1:135:A:LEU:H   | 1:135:A:LEU:HB3 | 10       | 0.27          |
| (1,763) | 1:92:A:ARG:HA   | 1:92:A:ARG:HD2  | 2        | 0.27          |
| (1,763) | 1:92:A:ARG:HA   | 1:92:A:ARG:HD3  | 2        | 0.27          |
| (1,722) | 1:72:A:GLN:HB2  | 1:87:A:THR:H    | 8        | 0.27          |
| (1,722) | 1:72:A:GLN:HB3  | 1:87:A:THR:H    | 8        | 0.27          |
| (1,684) | 1:61:A:LYS:H    | 1:61:A:LYS:HG2  | 9        | 0.27          |
| (1,684) | 1:61:A:LYS:H    | 1:61:A:LYS:HG3  | 9        | 0.27          |
| (1,560) | 1:9:A:LYS:HB2   | 1:10:A:VAL:H    | 7        | 0.27          |
| (1,560) | 1:9:A:LYS:HB3   | 1:10:A:VAL:H    | 7        | 0.27          |
| (1,560) | 1:9:A:LYS:HB2   | 1:10:A:VAL:H    | 8        | 0.27          |
| (1,560) | 1:9:A:LYS:HB3   | 1:10:A:VAL:H    | 8        | 0.27          |
| (1,467) | 1:115:A:PRO:HB3 | 1:117:A:PRO:HD2 | 4        | 0.27          |
| (1,434) | 1:69:A:TYR:HD1  | 1:90:A:LEU:HD11 | 3        | 0.27          |
| (1,434) | 1:69:A:TYR:HD1  | 1:90:A:LEU:HD12 | 3        | 0.27          |
| (1,434) | 1:69:A:TYR:HD1  | 1:90:A:LEU:HD13 | 3        | 0.27          |
| (1,434) | 1:69:A:TYR:HD2  | 1:90:A:LEU:HD11 | 3        | 0.27          |
| (1,434) | 1:69:A:TYR:HD2  | 1:90:A:LEU:HD12 | 3        | 0.27          |
| (1,434) | 1:69:A:TYR:HD2  | 1:90:A:LEU:HD13 | 3        | 0.27          |
| (1,366) | 1:83:A:LEU:HD11 | 1:109:A:CYS:H   | 7        | 0.27          |
| (1,366) | 1:83:A:LEU:HD12 | 1:109:A:CYS:H   | 7        | 0.27          |
| (1,366) | 1:83:A:LEU:HD13 | 1:109:A:CYS:H   | 7        | 0.27          |
| (1,366) | 1:83:A:LEU:HD11 | 1:109:A:CYS:H   | 8        | 0.27          |
| (1,366) | 1:83:A:LEU:HD12 | 1:109:A:CYS:H   | 8        | 0.27          |
| (1,366) | 1:83:A:LEU:HD13 | 1:109:A:CYS:H   | 8        | 0.27          |
| (1,330) | 1:96:A:ASN:HA   | 1:97:A:ALA:H    | 9        | 0.27          |
| (1,312) | 1:7:A:GLU:HA    | 1:8:A:LYS:H     | 9        | 0.27          |
| (1,291) | 1:85:A:THR:HB   | 1:86:A:ARG:H    | 3        | 0.27          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,287) | 1:79:A:LEU:HB3  | 1:81:A:THR:H    | 3        | 0.27          |
| (1,283) | 1:81:A:THR:H    | 1:82:A:ALA:HA   | 5        | 0.27          |
| (1,97)  | 1:26:A:THR:H    | 1:34:A:THR:H    | 10       | 0.27          |
| (1,63)  | 1:9:A:LYS:H     | 1:9:A:LYS:HA    | 5        | 0.27          |
| (1,828) | 1:133:A:LYS:H   | 1:133:A:LYS:HB2 | 9        | 0.26          |
| (1,828) | 1:133:A:LYS:H   | 1:133:A:LYS:HB3 | 9        | 0.26          |
| (1,807) | 1:111:A:LYS:HG2 | 1:112:A:LEU:H   | 4        | 0.26          |
| (1,807) | 1:111:A:LYS:HG3 | 1:112:A:LEU:H   | 4        | 0.26          |
| (1,734) | 1:76:A:GLU:H    | 1:76:A:GLU:HG2  | 5        | 0.26          |
| (1,734) | 1:76:A:GLU:H    | 1:76:A:GLU:HG3  | 5        | 0.26          |
| (1,667) | 1:52:A:ARG:HD2  | 1:53:A:CYS:H    | 5        | 0.26          |
| (1,667) | 1:52:A:ARG:HD3  | 1:53:A:CYS:H    | 5        | 0.26          |
| (1,646) | 1:46:A:GLN:H    | 1:46:A:GLN:HG2  | 7        | 0.26          |
| (1,646) | 1:46:A:GLN:H    | 1:46:A:GLN:HG3  | 7        | 0.26          |
| (1,629) | 1:38:A:THR:HB   | 1:48:A:MET:HG2  | 1        | 0.26          |
| (1,629) | 1:38:A:THR:HB   | 1:48:A:MET:HG3  | 1        | 0.26          |
| (1,605) | 1:26:A:THR:HA   | 1:33:A:GLY:HA2  | 9        | 0.26          |
| (1,605) | 1:26:A:THR:HA   | 1:33:A:GLY:HA3  | 9        | 0.26          |
| (1,602) | 1:26:A:THR:H    | 1:27:A:SER:HB2  | 7        | 0.26          |
| (1,602) | 1:26:A:THR:H    | 1:27:A:SER:HB3  | 7        | 0.26          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG21 | 3        | 0.26          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG22 | 3        | 0.26          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG23 | 3        | 0.26          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG21 | 4        | 0.26          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG22 | 4        | 0.26          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG23 | 4        | 0.26          |
| (1,467) | 1:115:A:PRO:HB3 | 1:117:A:PRO:HD2 | 2        | 0.26          |
| (1,440) | 1:20:A:TRP:HB3  | 1:20:A:TRP:HD1  | 8        | 0.26          |
| (1,366) | 1:83:A:LEU:HD11 | 1:109:A:CYS:H   | 1        | 0.26          |
| (1,366) | 1:83:A:LEU:HD12 | 1:109:A:CYS:H   | 1        | 0.26          |
| (1,366) | 1:83:A:LEU:HD13 | 1:109:A:CYS:H   | 1        | 0.26          |
| (1,297) | 1:26:A:THR:HB   | 1:32:A:LEU:HA   | 10       | 0.26          |
| (1,291) | 1:85:A:THR:HB   | 1:86:A:ARG:H    | 7        | 0.26          |
| (1,290) | 1:90:A:LEU:H    | 1:101:A:LYS:H   | 6        | 0.26          |
| (1,252) | 1:28:A:GLY:H    | 1:30:A:CYS:H    | 7        | 0.26          |
| (1,234) | 1:76:A:GLU:H    | 1:76:A:GLU:HB3  | 4        | 0.26          |
| (1,146) | 1:27:A:SER:HA   | 1:29:A:ASP:H    | 10       | 0.26          |
| (1,121) | 1:72:A:GLN:HG2  | 1:73:A:ALA:H    | 1        | 0.26          |
| (1,55)  | 1:18:A:TRP:H    | 1:18:A:TRP:HE3  | 2        | 0.26          |
| (1,25)  | 1:10:A:VAL:HB   | 1:11:A:LYS:H    | 3        | 0.26          |
| (1,25)  | 1:10:A:VAL:HB   | 1:11:A:LYS:H    | 5        | 0.26          |
| (1,17)  | 1:90:A:LEU:H    | 1:90:A:LEU:HG   | 2        | 0.26          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,17)  | 1:90:A:LEU:H    | 1:90:A:LEU:HG   | 7        | 0.26          |
| (1,833) | 1:135:A:LEU:HB2 | 1:136:A:ASP:H   | 1        | 0.25          |
| (1,833) | 1:135:A:LEU:HB3 | 1:136:A:ASP:H   | 1        | 0.25          |
| (1,807) | 1:111:A:LYS:HG2 | 1:112:A:LEU:H   | 7        | 0.25          |
| (1,807) | 1:111:A:LYS:HG3 | 1:112:A:LEU:H   | 7        | 0.25          |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD2  | 9        | 0.25          |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD3  | 9        | 0.25          |
| (1,622) | 1:33:A:GLY:HA2  | 1:34:A:THR:HG21 | 6        | 0.25          |
| (1,622) | 1:33:A:GLY:HA2  | 1:34:A:THR:HG22 | 6        | 0.25          |
| (1,622) | 1:33:A:GLY:HA2  | 1:34:A:THR:HG23 | 6        | 0.25          |
| (1,622) | 1:33:A:GLY:HA3  | 1:34:A:THR:HG21 | 6        | 0.25          |
| (1,622) | 1:33:A:GLY:HA3  | 1:34:A:THR:HG22 | 6        | 0.25          |
| (1,622) | 1:33:A:GLY:HA3  | 1:34:A:THR:HG23 | 6        | 0.25          |
| (1,602) | 1:26:A:THR:H    | 1:27:A:SER:HB2  | 4        | 0.25          |
| (1,602) | 1:26:A:THR:H    | 1:27:A:SER:HB3  | 4        | 0.25          |
| (1,297) | 1:26:A:THR:HB   | 1:32:A:LEU:HA   | 3        | 0.25          |
| (1,287) | 1:79:A:LEU:HB3  | 1:81:A:THR:H    | 8        | 0.25          |
| (1,148) | 1:62:A:GLN:H    | 1:63:A:PHE:HA   | 5        | 0.25          |
| (1,122) | 1:72:A:GLN:HG3  | 1:73:A:ALA:H    | 10       | 0.25          |
| (1,112) | 1:47:A:THR:HB   | 1:48:A:MET:H    | 2        | 0.25          |
| (1,97)  | 1:26:A:THR:H    | 1:34:A:THR:H    | 6        | 0.25          |
| (1,55)  | 1:18:A:TRP:H    | 1:18:A:TRP:HE3  | 5        | 0.25          |
| (1,48)  | 1:18:A:TRP:H    | 1:18:A:TRP:HE1  | 10       | 0.25          |
| (1,832) | 1:135:A:LEU:H   | 1:135:A:LEU:HB2 | 2        | 0.24          |
| (1,832) | 1:135:A:LEU:H   | 1:135:A:LEU:HB3 | 2        | 0.24          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD11 | 9        | 0.24          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD12 | 9        | 0.24          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD13 | 9        | 0.24          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD21 | 9        | 0.24          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD22 | 9        | 0.24          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD23 | 9        | 0.24          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD11 | 9        | 0.24          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD12 | 9        | 0.24          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD13 | 9        | 0.24          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD21 | 9        | 0.24          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD22 | 9        | 0.24          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD23 | 9        | 0.24          |
| (1,763) | 1:92:A:ARG:HA   | 1:92:A:ARG:HD2  | 3        | 0.24          |
| (1,763) | 1:92:A:ARG:HA   | 1:92:A:ARG:HD3  | 3        | 0.24          |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG2 | 3        | 0.24          |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG3 | 3        | 0.24          |
| (1,738) | 1:78:A:ASP:H    | 1:84:A:LYS:HG2  | 10       | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,738) | 1:78:A:ASP:H    | 1:84:A:LYS:HG3  | 10       | 0.24          |
| (1,667) | 1:52:A:ARG:HD2  | 1:53:A:CYS:H    | 9        | 0.24          |
| (1,667) | 1:52:A:ARG:HD3  | 1:53:A:CYS:H    | 9        | 0.24          |
| (1,316) | 1:89:A:SER:HA   | 1:90:A:LEU:HB3  | 7        | 0.24          |
| (1,250) | 1:30:A:CYS:H    | 1:55:A:ILE:HD11 | 9        | 0.24          |
| (1,250) | 1:30:A:CYS:H    | 1:55:A:ILE:HD12 | 9        | 0.24          |
| (1,250) | 1:30:A:CYS:H    | 1:55:A:ILE:HD13 | 9        | 0.24          |
| (1,201) | 1:78:A:ASP:HB2  | 1:83:A:LEU:H    | 9        | 0.24          |
| (1,148) | 1:62:A:GLN:H    | 1:63:A:PHE:HA   | 7        | 0.24          |
| (1,25)  | 1:10:A:VAL:HB   | 1:11:A:LYS:H    | 7        | 0.24          |
| (1,25)  | 1:10:A:VAL:HB   | 1:11:A:LYS:H    | 9        | 0.24          |
| (1,17)  | 1:90:A:LEU:H    | 1:90:A:LEU:HG   | 5        | 0.24          |
| (1,1)   | 1:78:A:ASP:H    | 1:85:A:THR:H    | 9        | 0.24          |
| (1,734) | 1:76:A:GLU:H    | 1:76:A:GLU:HG2  | 3        | 0.23          |
| (1,734) | 1:76:A:GLU:H    | 1:76:A:GLU:HG3  | 3        | 0.23          |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG2  | 10       | 0.23          |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG3  | 10       | 0.23          |
| (1,720) | 1:72:A:GLN:H    | 1:72:A:GLN:HG2  | 9        | 0.23          |
| (1,720) | 1:72:A:GLN:H    | 1:72:A:GLN:HG3  | 9        | 0.23          |
| (1,718) | 1:70:A:GLN:HG2  | 1:91:A:LYS:HG2  | 4        | 0.23          |
| (1,718) | 1:70:A:GLN:HG2  | 1:91:A:LYS:HG3  | 4        | 0.23          |
| (1,718) | 1:70:A:GLN:HG3  | 1:91:A:LYS:HG2  | 4        | 0.23          |
| (1,718) | 1:70:A:GLN:HG3  | 1:91:A:LYS:HG3  | 4        | 0.23          |
| (1,619) | 1:31:A:GLY:HA2  | 1:55:A:ILE:HG12 | 7        | 0.23          |
| (1,619) | 1:31:A:GLY:HA2  | 1:55:A:ILE:HG13 | 7        | 0.23          |
| (1,619) | 1:31:A:GLY:HA3  | 1:55:A:ILE:HG12 | 7        | 0.23          |
| (1,619) | 1:31:A:GLY:HA3  | 1:55:A:ILE:HG13 | 7        | 0.23          |
| (1,467) | 1:115:A:PRO:HB3 | 1:117:A:PRO:HD2 | 10       | 0.23          |
| (1,461) | 1:69:A:TYR:HD1  | 1:89:A:SER:HA   | 10       | 0.23          |
| (1,461) | 1:69:A:TYR:HD2  | 1:89:A:SER:HA   | 10       | 0.23          |
| (1,449) | 1:69:A:TYR:HA   | 1:69:A:TYR:HE1  | 1        | 0.23          |
| (1,449) | 1:69:A:TYR:HA   | 1:69:A:TYR:HE2  | 1        | 0.23          |
| (1,447) | 1:69:A:TYR:HE1  | 1:89:A:SER:HA   | 2        | 0.23          |
| (1,447) | 1:69:A:TYR:HE2  | 1:89:A:SER:HA   | 2        | 0.23          |
| (1,440) | 1:20:A:TRP:HB3  | 1:20:A:TRP:HD1  | 1        | 0.23          |
| (1,440) | 1:20:A:TRP:HB3  | 1:20:A:TRP:HD1  | 5        | 0.23          |
| (1,440) | 1:20:A:TRP:HB3  | 1:20:A:TRP:HD1  | 10       | 0.23          |
| (1,316) | 1:89:A:SER:HA   | 1:90:A:LEU:HB3  | 4        | 0.23          |
| (1,297) | 1:26:A:THR:HB   | 1:32:A:LEU:HA   | 1        | 0.23          |
| (1,296) | 1:103:A:VAL:HA  | 1:104:A:THR:HB  | 3        | 0.23          |
| (1,296) | 1:103:A:VAL:HA  | 1:104:A:THR:HB  | 10       | 0.23          |
| (1,233) | 1:78:A:ASP:HB2  | 1:80:A:ASN:H    | 9        | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,205) | 1:17:A:GLU:H    | 1:17:A:GLU:HB3  | 3        | 0.23          |
| (1,146) | 1:27:A:SER:HA   | 1:29:A:ASP:H    | 6        | 0.23          |
| (1,121) | 1:72:A:GLN:HG2  | 1:73:A:ALA:H    | 3        | 0.23          |
| (1,115) | 1:26:A:THR:H    | 1:27:A:SER:HB2  | 6        | 0.23          |
| (1,48)  | 1:18:A:TRP:H    | 1:18:A:TRP:HE1  | 9        | 0.23          |
| (1,36)  | 1:119:A:ALA:H   | 1:119:A:ALA:HA  | 3        | 0.23          |
| (1,36)  | 1:119:A:ALA:H   | 1:119:A:ALA:HA  | 7        | 0.23          |
| (1,17)  | 1:90:A:LEU:H    | 1:90:A:LEU:HG   | 3        | 0.23          |
| (1,828) | 1:133:A:LYS:H   | 1:133:A:LYS:HB2 | 1        | 0.22          |
| (1,828) | 1:133:A:LYS:H   | 1:133:A:LYS:HB3 | 1        | 0.22          |
| (1,778) | 1:98:A:GLU:HA   | 1:98:A:GLU:HG2  | 8        | 0.22          |
| (1,778) | 1:98:A:GLU:HA   | 1:98:A:GLU:HG3  | 8        | 0.22          |
| (1,746) | 1:83:A:LEU:HD11 | 1:108:A:PRO:HB2 | 1        | 0.22          |
| (1,746) | 1:83:A:LEU:HD11 | 1:108:A:PRO:HB3 | 1        | 0.22          |
| (1,746) | 1:83:A:LEU:HD12 | 1:108:A:PRO:HB2 | 1        | 0.22          |
| (1,746) | 1:83:A:LEU:HD12 | 1:108:A:PRO:HB3 | 1        | 0.22          |
| (1,746) | 1:83:A:LEU:HD13 | 1:108:A:PRO:HB2 | 1        | 0.22          |
| (1,746) | 1:83:A:LEU:HD13 | 1:108:A:PRO:HB3 | 1        | 0.22          |
| (1,746) | 1:83:A:LEU:HD11 | 1:108:A:PRO:HB2 | 10       | 0.22          |
| (1,746) | 1:83:A:LEU:HD11 | 1:108:A:PRO:HB3 | 10       | 0.22          |
| (1,746) | 1:83:A:LEU:HD12 | 1:108:A:PRO:HB2 | 10       | 0.22          |
| (1,746) | 1:83:A:LEU:HD12 | 1:108:A:PRO:HB3 | 10       | 0.22          |
| (1,746) | 1:83:A:LEU:HD13 | 1:108:A:PRO:HB2 | 10       | 0.22          |
| (1,746) | 1:83:A:LEU:HD13 | 1:108:A:PRO:HB3 | 10       | 0.22          |
| (1,738) | 1:78:A:ASP:H    | 1:84:A:LYS:HG2  | 3        | 0.22          |
| (1,738) | 1:78:A:ASP:H    | 1:84:A:LYS:HG3  | 3        | 0.22          |
| (1,667) | 1:52:A:ARG:HD2  | 1:53:A:CYS:H    | 1        | 0.22          |
| (1,667) | 1:52:A:ARG:HD3  | 1:53:A:CYS:H    | 1        | 0.22          |
| (1,574) | 1:15:A:CYS:H    | 1:15:A:CYS:HB2  | 3        | 0.22          |
| (1,574) | 1:15:A:CYS:H    | 1:15:A:CYS:HB3  | 3        | 0.22          |
| (1,551) | 1:6:A:PRO:HB2   | 1:7:A:GLU:H     | 1        | 0.22          |
| (1,551) | 1:6:A:PRO:HB3   | 1:7:A:GLU:H     | 1        | 0.22          |
| (1,551) | 1:6:A:PRO:HB2   | 1:7:A:GLU:H     | 2        | 0.22          |
| (1,551) | 1:6:A:PRO:HB3   | 1:7:A:GLU:H     | 2        | 0.22          |
| (1,551) | 1:6:A:PRO:HB2   | 1:7:A:GLU:H     | 10       | 0.22          |
| (1,551) | 1:6:A:PRO:HB3   | 1:7:A:GLU:H     | 10       | 0.22          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG21 | 5        | 0.22          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG22 | 5        | 0.22          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG23 | 5        | 0.22          |
| (1,467) | 1:115:A:PRO:HB3 | 1:117:A:PRO:HD2 | 7        | 0.22          |
| (1,440) | 1:20:A:TRP:HB3  | 1:20:A:TRP:HD1  | 4        | 0.22          |
| (1,374) | 1:46:A:GLN:H    | 1:47:A:THR:HG21 | 1        | 0.22          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,374) | 1:46:A:GLN:H   | 1:47:A:THR:HG22 | 1        | 0.22          |
| (1,374) | 1:46:A:GLN:H   | 1:47:A:THR:HG23 | 1        | 0.22          |
| (1,374) | 1:46:A:GLN:H   | 1:47:A:THR:HG21 | 5        | 0.22          |
| (1,374) | 1:46:A:GLN:H   | 1:47:A:THR:HG22 | 5        | 0.22          |
| (1,374) | 1:46:A:GLN:H   | 1:47:A:THR:HG23 | 5        | 0.22          |
| (1,374) | 1:46:A:GLN:H   | 1:47:A:THR:HG21 | 10       | 0.22          |
| (1,374) | 1:46:A:GLN:H   | 1:47:A:THR:HG22 | 10       | 0.22          |
| (1,374) | 1:46:A:GLN:H   | 1:47:A:THR:HG23 | 10       | 0.22          |
| (1,341) | 1:80:A:ASN:HB2 | 1:81:A:THR:HG21 | 6        | 0.22          |
| (1,341) | 1:80:A:ASN:HB2 | 1:81:A:THR:HG22 | 6        | 0.22          |
| (1,341) | 1:80:A:ASN:HB2 | 1:81:A:THR:HG23 | 6        | 0.22          |
| (1,316) | 1:89:A:SER:HA  | 1:90:A:LEU:HB3  | 5        | 0.22          |
| (1,296) | 1:103:A:VAL:HA | 1:104:A:THR:HB  | 2        | 0.22          |
| (1,296) | 1:103:A:VAL:HA | 1:104:A:THR:HB  | 9        | 0.22          |
| (1,283) | 1:81:A:THR:H   | 1:82:A:ALA:HA   | 7        | 0.22          |
| (1,262) | 1:27:A:SER:H   | 1:31:A:GLY:H    | 6        | 0.22          |
| (1,252) | 1:28:A:GLY:H   | 1:30:A:CYS:H    | 5        | 0.22          |
| (1,234) | 1:76:A:GLU:H   | 1:76:A:GLU:HB3  | 10       | 0.22          |
| (1,206) | 1:17:A:GLU:H   | 1:17:A:GLU:HB2  | 5        | 0.22          |
| (1,206) | 1:17:A:GLU:H   | 1:17:A:GLU:HB2  | 6        | 0.22          |
| (1,206) | 1:17:A:GLU:H   | 1:17:A:GLU:HB2  | 8        | 0.22          |
| (1,205) | 1:17:A:GLU:H   | 1:17:A:GLU:HB3  | 10       | 0.22          |
| (1,195) | 1:102:A:THR:HB | 1:103:A:VAL:H   | 4        | 0.22          |
| (1,133) | 1:90:A:LEU:HG  | 1:99:A:CYS:H    | 2        | 0.22          |
| (1,121) | 1:72:A:GLN:HG2 | 1:73:A:ALA:H    | 2        | 0.22          |
| (1,112) | 1:47:A:THR:HB  | 1:48:A:MET:H    | 4        | 0.22          |
| (1,68)  | 1:133:A:LYS:H  | 1:133:A:LYS:HA  | 3        | 0.22          |
| (1,68)  | 1:133:A:LYS:H  | 1:133:A:LYS:HA  | 5        | 0.22          |
| (1,43)  | 1:90:A:LEU:HB3 | 1:101:A:LYS:H   | 6        | 0.22          |
| (1,1)   | 1:78:A:ASP:H   | 1:85:A:THR:H    | 7        | 0.22          |
| (1,828) | 1:133:A:LYS:H  | 1:133:A:LYS:HB2 | 6        | 0.21          |
| (1,828) | 1:133:A:LYS:H  | 1:133:A:LYS:HB3 | 6        | 0.21          |
| (1,754) | 1:90:A:LEU:HB3 | 1:100:A:GLN:HG2 | 10       | 0.21          |
| (1,754) | 1:90:A:LEU:HB3 | 1:100:A:GLN:HG3 | 10       | 0.21          |
| (1,480) | 1:80:A:ASN:H   | 1:81:A:THR:HG21 | 1        | 0.21          |
| (1,480) | 1:80:A:ASN:H   | 1:81:A:THR:HG22 | 1        | 0.21          |
| (1,480) | 1:80:A:ASN:H   | 1:81:A:THR:HG23 | 1        | 0.21          |
| (1,461) | 1:69:A:TYR:HD1 | 1:89:A:SER:HA   | 1        | 0.21          |
| (1,461) | 1:69:A:TYR:HD2 | 1:89:A:SER:HA   | 1        | 0.21          |
| (1,447) | 1:69:A:TYR:HE1 | 1:89:A:SER:HA   | 8        | 0.21          |
| (1,447) | 1:69:A:TYR:HE2 | 1:89:A:SER:HA   | 8        | 0.21          |
| (1,440) | 1:20:A:TRP:HB3 | 1:20:A:TRP:HD1  | 6        | 0.21          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,440) | 1:20:A:TRP:HB3 | 1:20:A:TRP:HD1  | 7        | 0.21          |
| (1,440) | 1:20:A:TRP:HB3 | 1:20:A:TRP:HD1  | 9        | 0.21          |
| (1,348) | 1:94:A:LEU:HG  | 1:95:A:HIS:H    | 10       | 0.21          |
| (1,340) | 1:86:A:ARG:H   | 1:105:A:ILE:HB  | 1        | 0.21          |
| (1,316) | 1:89:A:SER:HA  | 1:90:A:LEU:HB3  | 3        | 0.21          |
| (1,291) | 1:85:A:THR:HB  | 1:86:A:ARG:H    | 2        | 0.21          |
| (1,291) | 1:85:A:THR:HB  | 1:86:A:ARG:H    | 8        | 0.21          |
| (1,206) | 1:17:A:GLU:H   | 1:17:A:GLU:HB2  | 1        | 0.21          |
| (1,152) | 1:43:A:GLU:HA  | 1:44:A:CYS:H    | 8        | 0.21          |
| (1,112) | 1:47:A:THR:HB  | 1:48:A:MET:H    | 8        | 0.21          |
| (1,109) | 1:8:A:LYS:H    | 1:8:A:LYS:HA    | 4        | 0.21          |
| (1,109) | 1:8:A:LYS:H    | 1:8:A:LYS:HA    | 5        | 0.21          |
| (1,87)  | 1:82:A:ALA:H   | 1:83:A:LEU:HG   | 9        | 0.21          |
| (1,68)  | 1:133:A:LYS:H  | 1:133:A:LYS:HA  | 8        | 0.21          |
| (1,36)  | 1:119:A:ALA:H  | 1:119:A:ALA:HA  | 8        | 0.21          |
| (1,721) | 1:72:A:GLN:HA  | 1:72:A:GLN:HG2  | 8        | 0.2           |
| (1,721) | 1:72:A:GLN:HA  | 1:72:A:GLN:HG3  | 8        | 0.2           |
| (1,667) | 1:52:A:ARG:HD2 | 1:53:A:CYS:H    | 6        | 0.2           |
| (1,667) | 1:52:A:ARG:HD3 | 1:53:A:CYS:H    | 6        | 0.2           |
| (1,605) | 1:26:A:THR:HA  | 1:33:A:GLY:HA2  | 6        | 0.2           |
| (1,605) | 1:26:A:THR:HA  | 1:33:A:GLY:HA3  | 6        | 0.2           |
| (1,560) | 1:9:A:LYS:HB2  | 1:10:A:VAL:H    | 2        | 0.2           |
| (1,560) | 1:9:A:LYS:HB3  | 1:10:A:VAL:H    | 2        | 0.2           |
| (1,551) | 1:6:A:PRO:HB2  | 1:7:A:GLU:H     | 6        | 0.2           |
| (1,551) | 1:6:A:PRO:HB3  | 1:7:A:GLU:H     | 6        | 0.2           |
| (1,551) | 1:6:A:PRO:HB2  | 1:7:A:GLU:H     | 7        | 0.2           |
| (1,551) | 1:6:A:PRO:HB3  | 1:7:A:GLU:H     | 7        | 0.2           |
| (1,471) | 1:54:A:LYS:H   | 1:54:A:LYS:HG2  | 6        | 0.2           |
| (1,317) | 1:90:A:LEU:HB3 | 1:101:A:LYS:HA  | 6        | 0.2           |
| (1,287) | 1:79:A:LEU:HB3 | 1:81:A:THR:H    | 1        | 0.2           |
| (1,283) | 1:81:A:THR:H   | 1:82:A:ALA:HA   | 8        | 0.2           |
| (1,250) | 1:30:A:CYS:H   | 1:55:A:ILE:HD11 | 6        | 0.2           |
| (1,250) | 1:30:A:CYS:H   | 1:55:A:ILE:HD12 | 6        | 0.2           |
| (1,250) | 1:30:A:CYS:H   | 1:55:A:ILE:HD13 | 6        | 0.2           |
| (1,233) | 1:78:A:ASP:HB2 | 1:80:A:ASN:H    | 4        | 0.2           |
| (1,121) | 1:72:A:GLN:HG2 | 1:73:A:ALA:H    | 5        | 0.2           |
| (1,68)  | 1:133:A:LYS:H  | 1:133:A:LYS:HA  | 7        | 0.2           |
| (1,55)  | 1:18:A:TRP:H   | 1:18:A:TRP:HE3  | 1        | 0.2           |
| (1,808) | 1:112:A:LEU:H  | 1:112:A:LEU:HB2 | 8        | 0.19          |
| (1,808) | 1:112:A:LEU:H  | 1:112:A:LEU:HB3 | 8        | 0.19          |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG2  | 3        | 0.19          |
| (1,745) | 1:83:A:LEU:HA  | 1:84:A:LYS:HG3  | 3        | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,722) | 1:72:A:GLN:HB2  | 1:87:A:THR:H    | 1        | 0.19          |
| (1,722) | 1:72:A:GLN:HB3  | 1:87:A:THR:H    | 1        | 0.19          |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG2  | 6        | 0.19          |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG3  | 6        | 0.19          |
| (1,660) | 1:51:A:GLN:HA   | 1:52:A:ARG:HG2  | 3        | 0.19          |
| (1,660) | 1:51:A:GLN:HA   | 1:52:A:ARG:HG3  | 3        | 0.19          |
| (1,589) | 1:19:A:GLN:HG2  | 1:20:A:TRP:H    | 4        | 0.19          |
| (1,589) | 1:19:A:GLN:HG3  | 1:20:A:TRP:H    | 4        | 0.19          |
| (1,467) | 1:115:A:PRO:HB3 | 1:117:A:PRO:HD2 | 5        | 0.19          |
| (1,307) | 1:26:A:THR:HG21 | 1:27:A:SER:HB2  | 5        | 0.19          |
| (1,307) | 1:26:A:THR:HG22 | 1:27:A:SER:HB2  | 5        | 0.19          |
| (1,307) | 1:26:A:THR:HG23 | 1:27:A:SER:HB2  | 5        | 0.19          |
| (1,296) | 1:103:A:VAL:HA  | 1:104:A:THR:HB  | 4        | 0.19          |
| (1,296) | 1:103:A:VAL:HA  | 1:104:A:THR:HB  | 5        | 0.19          |
| (1,296) | 1:103:A:VAL:HA  | 1:104:A:THR:HB  | 6        | 0.19          |
| (1,296) | 1:103:A:VAL:HA  | 1:104:A:THR:HB  | 7        | 0.19          |
| (1,283) | 1:81:A:THR:H    | 1:82:A:ALA:HA   | 3        | 0.19          |
| (1,252) | 1:28:A:GLY:H    | 1:30:A:CYS:H    | 2        | 0.19          |
| (1,234) | 1:76:A:GLU:H    | 1:76:A:GLU:HB3  | 6        | 0.19          |
| (1,204) | 1:105:A:ILE:HB  | 1:106:A:SER:H   | 7        | 0.19          |
| (1,195) | 1:102:A:THR:HB  | 1:103:A:VAL:H   | 10       | 0.19          |
| (1,188) | 1:12:A:LYS:HA   | 1:13:A:SER:H    | 10       | 0.19          |
| (1,148) | 1:62:A:GLN:H    | 1:63:A:PHE:HA   | 9        | 0.19          |
| (1,147) | 1:61:A:LYS:HA   | 1:62:A:GLN:H    | 5        | 0.19          |
| (1,112) | 1:47:A:THR:HB   | 1:48:A:MET:H    | 10       | 0.19          |
| (1,109) | 1:8:A:LYS:H     | 1:8:A:LYS:HA    | 8        | 0.19          |
| (1,87)  | 1:82:A:ALA:H    | 1:83:A:LEU:HG   | 7        | 0.19          |
| (1,17)  | 1:90:A:LEU:H    | 1:90:A:LEU:HG   | 4        | 0.19          |
| (1,1)   | 1:78:A:ASP:H    | 1:85:A:THR:H    | 8        | 0.19          |
| (1,833) | 1:135:A:LEU:HB2 | 1:136:A:ASP:H   | 7        | 0.18          |
| (1,833) | 1:135:A:LEU:HB3 | 1:136:A:ASP:H   | 7        | 0.18          |
| (1,828) | 1:133:A:LYS:H   | 1:133:A:LYS:HB2 | 10       | 0.18          |
| (1,828) | 1:133:A:LYS:H   | 1:133:A:LYS:HB3 | 10       | 0.18          |
| (1,827) | 1:132:A:GLU:HB2 | 1:133:A:LYS:H   | 1        | 0.18          |
| (1,827) | 1:132:A:GLU:HB3 | 1:133:A:LYS:H   | 1        | 0.18          |
| (1,825) | 1:132:A:GLU:H   | 1:132:A:GLU:HB2 | 7        | 0.18          |
| (1,825) | 1:132:A:GLU:H   | 1:132:A:GLU:HB3 | 7        | 0.18          |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG2 | 6        | 0.18          |
| (1,754) | 1:90:A:LEU:HB3  | 1:100:A:GLN:HG3 | 6        | 0.18          |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG2  | 7        | 0.18          |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG3  | 7        | 0.18          |
| (1,659) | 1:49:A:LYS:HG2  | 1:50:A:THR:H    | 10       | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,659) | 1:49:A:LYS:HG3  | 1:50:A:THR:H    | 10       | 0.18          |
| (1,608) | 1:26:A:THR:HG21 | 1:27:A:SER:HB2  | 1        | 0.18          |
| (1,608) | 1:26:A:THR:HG21 | 1:27:A:SER:HB3  | 1        | 0.18          |
| (1,608) | 1:26:A:THR:HG22 | 1:27:A:SER:HB2  | 1        | 0.18          |
| (1,608) | 1:26:A:THR:HG22 | 1:27:A:SER:HB3  | 1        | 0.18          |
| (1,608) | 1:26:A:THR:HG23 | 1:27:A:SER:HB2  | 1        | 0.18          |
| (1,608) | 1:26:A:THR:HG23 | 1:27:A:SER:HB3  | 1        | 0.18          |
| (1,571) | 1:13:A:SER:HA   | 1:14:A:ASP:HB2  | 2        | 0.18          |
| (1,571) | 1:13:A:SER:HA   | 1:14:A:ASP:HB3  | 2        | 0.18          |
| (1,440) | 1:20:A:TRP:HB3  | 1:20:A:TRP:HD1  | 3        | 0.18          |
| (1,307) | 1:26:A:THR:HG21 | 1:27:A:SER:HB2  | 9        | 0.18          |
| (1,307) | 1:26:A:THR:HG22 | 1:27:A:SER:HB2  | 9        | 0.18          |
| (1,307) | 1:26:A:THR:HG23 | 1:27:A:SER:HB2  | 9        | 0.18          |
| (1,283) | 1:81:A:THR:H    | 1:82:A:ALA:HA   | 2        | 0.18          |
| (1,271) | 1:40:A:THR:HB   | 1:41:A:GLY:H    | 2        | 0.18          |
| (1,204) | 1:105:A:ILE:HB  | 1:106:A:SER:H   | 9        | 0.18          |
| (1,148) | 1:62:A:GLN:H    | 1:63:A:PHE:HA   | 2        | 0.18          |
| (1,148) | 1:62:A:GLN:H    | 1:63:A:PHE:HA   | 4        | 0.18          |
| (1,22)  | 1:78:A:ASP:HB2  | 1:79:A:LEU:H    | 3        | 0.18          |
| (1,827) | 1:132:A:GLU:HB2 | 1:133:A:LYS:H   | 6        | 0.17          |
| (1,827) | 1:132:A:GLU:HB3 | 1:133:A:LYS:H   | 6        | 0.17          |
| (1,766) | 1:92:A:ARG:HG2  | 1:93:A:ALA:H    | 5        | 0.17          |
| (1,766) | 1:92:A:ARG:HG3  | 1:93:A:ALA:H    | 5        | 0.17          |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG2  | 1        | 0.17          |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG3  | 1        | 0.17          |
| (1,659) | 1:49:A:LYS:HG2  | 1:50:A:THR:H    | 8        | 0.17          |
| (1,659) | 1:49:A:LYS:HG3  | 1:50:A:THR:H    | 8        | 0.17          |
| (1,605) | 1:26:A:THR:HA   | 1:33:A:GLY:HA2  | 10       | 0.17          |
| (1,605) | 1:26:A:THR:HA   | 1:33:A:GLY:HA3  | 10       | 0.17          |
| (1,468) | 1:115:A:PRO:HB3 | 1:117:A:PRO:HD3 | 3        | 0.17          |
| (1,449) | 1:69:A:TYR:HA   | 1:69:A:TYR:HE1  | 5        | 0.17          |
| (1,449) | 1:69:A:TYR:HA   | 1:69:A:TYR:HE2  | 5        | 0.17          |
| (1,447) | 1:69:A:TYR:HE1  | 1:89:A:SER:HA   | 6        | 0.17          |
| (1,447) | 1:69:A:TYR:HE2  | 1:89:A:SER:HA   | 6        | 0.17          |
| (1,374) | 1:46:A:GLN:H    | 1:47:A:THR:HG21 | 3        | 0.17          |
| (1,374) | 1:46:A:GLN:H    | 1:47:A:THR:HG22 | 3        | 0.17          |
| (1,374) | 1:46:A:GLN:H    | 1:47:A:THR:HG23 | 3        | 0.17          |
| (1,366) | 1:83:A:LEU:HD11 | 1:109:A:CYS:H   | 6        | 0.17          |
| (1,366) | 1:83:A:LEU:HD12 | 1:109:A:CYS:H   | 6        | 0.17          |
| (1,366) | 1:83:A:LEU:HD13 | 1:109:A:CYS:H   | 6        | 0.17          |
| (1,330) | 1:96:A:ASN:HA   | 1:97:A:ALA:H    | 4        | 0.17          |
| (1,296) | 1:103:A:VAL:HA  | 1:104:A:THR:HB  | 8        | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,276) | 1:63:A:PHE:HB2  | 1:64:A:GLY:H    | 7        | 0.17          |
| (1,227) | 1:26:A:THR:HB   | 1:27:A:SER:H    | 6        | 0.17          |
| (1,205) | 1:17:A:GLU:H    | 1:17:A:GLU:HB3  | 9        | 0.17          |
| (1,204) | 1:105:A:ILE:HB  | 1:106:A:SER:H   | 5        | 0.17          |
| (1,167) | 1:97:A:ALA:HB1  | 1:98:A:GLU:H    | 1        | 0.17          |
| (1,167) | 1:97:A:ALA:HB2  | 1:98:A:GLU:H    | 1        | 0.17          |
| (1,167) | 1:97:A:ALA:HB3  | 1:98:A:GLU:H    | 1        | 0.17          |
| (1,166) | 1:46:A:GLN:H    | 1:46:A:GLN:HG3  | 3        | 0.17          |
| (1,97)  | 1:26:A:THR:H    | 1:34:A:THR:H    | 8        | 0.17          |
| (1,87)  | 1:82:A:ALA:H    | 1:83:A:LEU:HG   | 1        | 0.17          |
| (1,55)  | 1:18:A:TRP:H    | 1:18:A:TRP:HE3  | 10       | 0.17          |
| (1,36)  | 1:119:A:ALA:H   | 1:119:A:ALA:HA  | 5        | 0.17          |
| (1,821) | 1:130:A:LYS:H   | 1:130:A:LYS:HB2 | 10       | 0.16          |
| (1,821) | 1:130:A:LYS:H   | 1:130:A:LYS:HB3 | 10       | 0.16          |
| (1,808) | 1:112:A:LEU:H   | 1:112:A:LEU:HB2 | 2        | 0.16          |
| (1,808) | 1:112:A:LEU:H   | 1:112:A:LEU:HB3 | 2        | 0.16          |
| (1,807) | 1:111:A:LYS:HG2 | 1:112:A:LEU:H   | 2        | 0.16          |
| (1,807) | 1:111:A:LYS:HG3 | 1:112:A:LEU:H   | 2        | 0.16          |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG2  | 2        | 0.16          |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG3  | 2        | 0.16          |
| (1,692) | 1:62:A:GLN:HB2  | 1:63:A:PHE:HA   | 2        | 0.16          |
| (1,692) | 1:62:A:GLN:HB3  | 1:63:A:PHE:HA   | 2        | 0.16          |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD2  | 1        | 0.16          |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD3  | 1        | 0.16          |
| (1,660) | 1:51:A:GLN:HA   | 1:52:A:ARG:HG2  | 5        | 0.16          |
| (1,660) | 1:51:A:GLN:HA   | 1:52:A:ARG:HG3  | 5        | 0.16          |
| (1,629) | 1:38:A:THR:HB   | 1:48:A:MET:HG2  | 10       | 0.16          |
| (1,629) | 1:38:A:THR:HB   | 1:48:A:MET:HG3  | 10       | 0.16          |
| (1,589) | 1:19:A:GLN:HG2  | 1:20:A:TRP:H    | 1        | 0.16          |
| (1,589) | 1:19:A:GLN:HG3  | 1:20:A:TRP:H    | 1        | 0.16          |
| (1,574) | 1:15:A:CYS:H    | 1:15:A:CYS:HB2  | 8        | 0.16          |
| (1,574) | 1:15:A:CYS:H    | 1:15:A:CYS:HB3  | 8        | 0.16          |
| (1,562) | 1:9:A:LYS:HG2   | 1:10:A:VAL:H    | 3        | 0.16          |
| (1,562) | 1:9:A:LYS:HG3   | 1:10:A:VAL:H    | 3        | 0.16          |
| (1,557) | 1:8:A:LYS:HG2   | 1:9:A:LYS:H     | 7        | 0.16          |
| (1,557) | 1:8:A:LYS:HG3   | 1:9:A:LYS:H     | 7        | 0.16          |
| (1,554) | 1:8:A:LYS:H     | 1:8:A:LYS:HB2   | 7        | 0.16          |
| (1,554) | 1:8:A:LYS:H     | 1:8:A:LYS:HB3   | 7        | 0.16          |
| (1,531) | 1:30:A:CYS:H    | 1:55:A:ILE:HG21 | 5        | 0.16          |
| (1,531) | 1:30:A:CYS:H    | 1:55:A:ILE:HG22 | 5        | 0.16          |
| (1,531) | 1:30:A:CYS:H    | 1:55:A:ILE:HG23 | 5        | 0.16          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG21 | 7        | 0.16          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,480) | 1:80:A:ASN:H     | 1:81:A:THR:HG22 | 7        | 0.16          |
| (1,480) | 1:80:A:ASN:H     | 1:81:A:THR:HG23 | 7        | 0.16          |
| (1,478) | 1:104:A:THR:HG21 | 1:105:A:ILE:H   | 1        | 0.16          |
| (1,478) | 1:104:A:THR:HG22 | 1:105:A:ILE:H   | 1        | 0.16          |
| (1,478) | 1:104:A:THR:HG23 | 1:105:A:ILE:H   | 1        | 0.16          |
| (1,467) | 1:115:A:PRO:HB3  | 1:117:A:PRO:HD2 | 8        | 0.16          |
| (1,467) | 1:115:A:PRO:HB3  | 1:117:A:PRO:HD2 | 9        | 0.16          |
| (1,449) | 1:69:A:TYR:HA    | 1:69:A:TYR:HE1  | 4        | 0.16          |
| (1,449) | 1:69:A:TYR:HA    | 1:69:A:TYR:HE2  | 4        | 0.16          |
| (1,366) | 1:83:A:LEU:HD11  | 1:109:A:CYS:H   | 10       | 0.16          |
| (1,366) | 1:83:A:LEU:HD12  | 1:109:A:CYS:H   | 10       | 0.16          |
| (1,366) | 1:83:A:LEU:HD13  | 1:109:A:CYS:H   | 10       | 0.16          |
| (1,330) | 1:96:A:ASN:HA    | 1:97:A:ALA:H    | 6        | 0.16          |
| (1,316) | 1:89:A:SER:HA    | 1:90:A:LEU:HB3  | 10       | 0.16          |
| (1,296) | 1:103:A:VAL:HA   | 1:104:A:THR:HB  | 1        | 0.16          |
| (1,292) | 1:50:A:THR:HB    | 1:51:A:GLN:H    | 3        | 0.16          |
| (1,287) | 1:79:A:LEU:HB3   | 1:81:A:THR:H    | 4        | 0.16          |
| (1,234) | 1:76:A:GLU:H     | 1:76:A:GLU:HB3  | 7        | 0.16          |
| (1,233) | 1:78:A:ASP:HB2   | 1:80:A:ASN:H    | 6        | 0.16          |
| (1,211) | 1:83:A:LEU:HG    | 1:109:A:CYS:H   | 8        | 0.16          |
| (1,204) | 1:105:A:ILE:HB   | 1:106:A:SER:H   | 1        | 0.16          |
| (1,166) | 1:46:A:GLN:H     | 1:46:A:GLN:HG3  | 2        | 0.16          |
| (1,133) | 1:90:A:LEU:HG    | 1:99:A:CYS:H    | 1        | 0.16          |
| (1,100) | 1:59:A:TRP:H     | 1:59:A:TRP:HD1  | 6        | 0.16          |
| (1,85)  | 1:85:A:THR:HG21  | 1:86:A:ARG:H    | 10       | 0.16          |
| (1,85)  | 1:85:A:THR:HG22  | 1:86:A:ARG:H    | 10       | 0.16          |
| (1,85)  | 1:85:A:THR:HG23  | 1:86:A:ARG:H    | 10       | 0.16          |
| (1,67)  | 1:111:A:LYS:HA   | 1:112:A:LEU:H   | 4        | 0.16          |
| (1,55)  | 1:18:A:TRP:H     | 1:18:A:TRP:HE3  | 8        | 0.16          |
| (1,36)  | 1:119:A:ALA:H    | 1:119:A:ALA:HA  | 1        | 0.16          |
| (1,36)  | 1:119:A:ALA:H    | 1:119:A:ALA:HA  | 9        | 0.16          |
| (1,791) | 1:100:A:GLN:HG2  | 1:102:A:THR:H   | 6        | 0.15          |
| (1,791) | 1:100:A:GLN:HG3  | 1:102:A:THR:H   | 6        | 0.15          |
| (1,721) | 1:72:A:GLN:HA    | 1:72:A:GLN:HG2  | 3        | 0.15          |
| (1,721) | 1:72:A:GLN:HA    | 1:72:A:GLN:HG3  | 3        | 0.15          |
| (1,681) | 1:60:A:LYS:HA    | 1:60:A:LYS:HD2  | 2        | 0.15          |
| (1,681) | 1:60:A:LYS:HA    | 1:60:A:LYS:HD3  | 2        | 0.15          |
| (1,671) | 1:54:A:LYS:HG2   | 1:55:A:ILE:H    | 3        | 0.15          |
| (1,671) | 1:54:A:LYS:HG3   | 1:55:A:ILE:H    | 3        | 0.15          |
| (1,605) | 1:26:A:THR:HA    | 1:33:A:GLY:HA2  | 2        | 0.15          |
| (1,605) | 1:26:A:THR:HA    | 1:33:A:GLY:HA3  | 2        | 0.15          |
| (1,602) | 1:26:A:THR:H     | 1:27:A:SER:HB2  | 2        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,602) | 1:26:A:THR:H    | 1:27:A:SER:HB3  | 2        | 0.15          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG21 | 8        | 0.15          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG22 | 8        | 0.15          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG23 | 8        | 0.15          |
| (1,420) | 1:35:A:ARG:H    | 1:36:A:GLU:HA   | 6        | 0.15          |
| (1,292) | 1:50:A:THR:HB   | 1:51:A:GLN:H    | 8        | 0.15          |
| (1,291) | 1:85:A:THR:HB   | 1:86:A:ARG:H    | 5        | 0.15          |
| (1,276) | 1:63:A:PHE:HB2  | 1:64:A:GLY:H    | 9        | 0.15          |
| (1,250) | 1:30:A:CYS:H    | 1:55:A:ILE:HD11 | 8        | 0.15          |
| (1,250) | 1:30:A:CYS:H    | 1:55:A:ILE:HD12 | 8        | 0.15          |
| (1,250) | 1:30:A:CYS:H    | 1:55:A:ILE:HD13 | 8        | 0.15          |
| (1,109) | 1:8:A:LYS:H     | 1:8:A:LYS:HA    | 6        | 0.15          |
| (1,87)  | 1:82:A:ALA:H    | 1:83:A:LEU:HG   | 8        | 0.15          |
| (1,85)  | 1:85:A:THR:HG21 | 1:86:A:ARG:H    | 1        | 0.15          |
| (1,85)  | 1:85:A:THR:HG22 | 1:86:A:ARG:H    | 1        | 0.15          |
| (1,85)  | 1:85:A:THR:HG23 | 1:86:A:ARG:H    | 1        | 0.15          |
| (1,70)  | 1:104:A:THR:HB  | 1:105:A:ILE:H   | 9        | 0.15          |
| (1,68)  | 1:133:A:LYS:H   | 1:133:A:LYS:HA  | 2        | 0.15          |
| (1,55)  | 1:18:A:TRP:H    | 1:18:A:TRP:HE3  | 6        | 0.15          |
| (1,48)  | 1:18:A:TRP:H    | 1:18:A:TRP:HE1  | 2        | 0.15          |
| (1,40)  | 1:113:A:THR:HB  | 1:114:A:LYS:H   | 10       | 0.15          |
| (1,37)  | 1:11:A:LYS:HA   | 1:12:A:LYS:H    | 5        | 0.15          |
| (1,36)  | 1:119:A:ALA:H   | 1:119:A:ALA:HA  | 2        | 0.15          |
| (1,22)  | 1:78:A:ASP:HB2  | 1:79:A:LEU:H    | 5        | 0.15          |
| (1,2)   | 1:59:A:TRP:H    | 1:59:A:TRP:HE1  | 1        | 0.15          |
| (1,810) | 1:113:A:THR:HA  | 1:115:A:PRO:HD2 | 1        | 0.14          |
| (1,810) | 1:113:A:THR:HA  | 1:115:A:PRO:HD3 | 1        | 0.14          |
| (1,810) | 1:113:A:THR:HA  | 1:115:A:PRO:HD2 | 3        | 0.14          |
| (1,810) | 1:113:A:THR:HA  | 1:115:A:PRO:HD3 | 3        | 0.14          |
| (1,805) | 1:111:A:LYS:H   | 1:111:A:LYS:HB2 | 6        | 0.14          |
| (1,805) | 1:111:A:LYS:H   | 1:111:A:LYS:HB3 | 6        | 0.14          |
| (1,741) | 1:79:A:LEU:HB2  | 1:81:A:THR:H    | 5        | 0.14          |
| (1,741) | 1:79:A:LEU:HB3  | 1:81:A:THR:H    | 5        | 0.14          |
| (1,738) | 1:78:A:ASP:H    | 1:84:A:LYS:HG2  | 6        | 0.14          |
| (1,738) | 1:78:A:ASP:H    | 1:84:A:LYS:HG3  | 6        | 0.14          |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG2  | 5        | 0.14          |
| (1,721) | 1:72:A:GLN:HA   | 1:72:A:GLN:HG3  | 5        | 0.14          |
| (1,708) | 1:68:A:LYS:H    | 1:68:A:LYS:HG2  | 3        | 0.14          |
| (1,708) | 1:68:A:LYS:H    | 1:68:A:LYS:HG3  | 3        | 0.14          |
| (1,667) | 1:52:A:ARG:HD2  | 1:53:A:CYS:H    | 7        | 0.14          |
| (1,667) | 1:52:A:ARG:HD3  | 1:53:A:CYS:H    | 7        | 0.14          |
| (1,644) | 1:45:A:LYS:HG2  | 1:46:A:GLN:H    | 3        | 0.14          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,644) | 1:45:A:LYS:HG3  | 1:46:A:GLN:H     | 3        | 0.14          |
| (1,468) | 1:115:A:PRO:HB3 | 1:117:A:PRO:HD3  | 1        | 0.14          |
| (1,447) | 1:69:A:TYR:HE1  | 1:89:A:SER:HA    | 4        | 0.14          |
| (1,447) | 1:69:A:TYR:HE2  | 1:89:A:SER:HA    | 4        | 0.14          |
| (1,351) | 1:90:A:LEU:HG   | 1:101:A:LYS:HA   | 9        | 0.14          |
| (1,307) | 1:26:A:THR:HG21 | 1:27:A:SER:HB2   | 10       | 0.14          |
| (1,307) | 1:26:A:THR:HG22 | 1:27:A:SER:HB2   | 10       | 0.14          |
| (1,307) | 1:26:A:THR:HG23 | 1:27:A:SER:HB2   | 10       | 0.14          |
| (1,286) | 1:79:A:LEU:HB2  | 1:81:A:THR:H     | 2        | 0.14          |
| (1,283) | 1:81:A:THR:H    | 1:82:A:ALA:HA    | 10       | 0.14          |
| (1,266) | 1:63:A:PHE:HA   | 1:64:A:GLY:H     | 1        | 0.14          |
| (1,246) | 1:28:A:GLY:HA3  | 1:30:A:CYS:H     | 6        | 0.14          |
| (1,234) | 1:76:A:GLU:H    | 1:76:A:GLU:HB3   | 1        | 0.14          |
| (1,231) | 1:80:A:ASN:H    | 1:80:A:ASN:HB3   | 1        | 0.14          |
| (1,231) | 1:80:A:ASN:H    | 1:80:A:ASN:HB3   | 10       | 0.14          |
| (1,195) | 1:102:A:THR:HB  | 1:103:A:VAL:H    | 6        | 0.14          |
| (1,195) | 1:102:A:THR:HB  | 1:103:A:VAL:H    | 7        | 0.14          |
| (1,133) | 1:90:A:LEU:HG   | 1:99:A:CYS:H     | 7        | 0.14          |
| (1,123) | 1:71:A:PHE:HB2  | 1:72:A:GLN:H     | 9        | 0.14          |
| (1,77)  | 1:115:A:PRO:HB2 | 1:116:A:LYS:H    | 7        | 0.14          |
| (1,70)  | 1:104:A:THR:HB  | 1:105:A:ILE:H    | 1        | 0.14          |
| (1,68)  | 1:133:A:LYS:H   | 1:133:A:LYS:HA   | 4        | 0.14          |
| (1,61)  | 1:13:A:SER:HA   | 1:14:A:ASP:H     | 3        | 0.14          |
| (1,55)  | 1:18:A:TRP:H    | 1:18:A:TRP:HE3   | 4        | 0.14          |
| (1,22)  | 1:78:A:ASP:HB2  | 1:79:A:LEU:H     | 2        | 0.14          |
| (1,22)  | 1:78:A:ASP:HB2  | 1:79:A:LEU:H     | 4        | 0.14          |
| (1,22)  | 1:78:A:ASP:HB2  | 1:79:A:LEU:H     | 8        | 0.14          |
| (1,22)  | 1:78:A:ASP:HB2  | 1:79:A:LEU:H     | 10       | 0.14          |
| (1,17)  | 1:90:A:LEU:H    | 1:90:A:LEU:HG    | 10       | 0.14          |
| (1,1)   | 1:78:A:ASP:H    | 1:85:A:THR:H     | 6        | 0.14          |
| (1,800) | 1:101:A:LYS:HG2 | 1:102:A:THR:HG21 | 5        | 0.13          |
| (1,800) | 1:101:A:LYS:HG2 | 1:102:A:THR:HG22 | 5        | 0.13          |
| (1,800) | 1:101:A:LYS:HG2 | 1:102:A:THR:HG23 | 5        | 0.13          |
| (1,800) | 1:101:A:LYS:HG3 | 1:102:A:THR:HG21 | 5        | 0.13          |
| (1,800) | 1:101:A:LYS:HG3 | 1:102:A:THR:HG22 | 5        | 0.13          |
| (1,800) | 1:101:A:LYS:HG3 | 1:102:A:THR:HG23 | 5        | 0.13          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD11  | 2        | 0.13          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD12  | 2        | 0.13          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD13  | 2        | 0.13          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD21  | 2        | 0.13          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD22  | 2        | 0.13          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD23  | 2        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD11 | 2        | 0.13          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD12 | 2        | 0.13          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD13 | 2        | 0.13          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD21 | 2        | 0.13          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD22 | 2        | 0.13          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD23 | 2        | 0.13          |
| (1,763) | 1:92:A:ARG:HA   | 1:92:A:ARG:HD2  | 8        | 0.13          |
| (1,763) | 1:92:A:ARG:HA   | 1:92:A:ARG:HD3  | 8        | 0.13          |
| (1,722) | 1:72:A:GLN:HB2  | 1:87:A:THR:H    | 6        | 0.13          |
| (1,722) | 1:72:A:GLN:HB3  | 1:87:A:THR:H    | 6        | 0.13          |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD2  | 5        | 0.13          |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD3  | 5        | 0.13          |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD2  | 6        | 0.13          |
| (1,681) | 1:60:A:LYS:HA   | 1:60:A:LYS:HD3  | 6        | 0.13          |
| (1,667) | 1:52:A:ARG:HD2  | 1:53:A:CYS:H    | 2        | 0.13          |
| (1,667) | 1:52:A:ARG:HD3  | 1:53:A:CYS:H    | 2        | 0.13          |
| (1,608) | 1:26:A:THR:HG21 | 1:27:A:SER:HB2  | 5        | 0.13          |
| (1,608) | 1:26:A:THR:HG21 | 1:27:A:SER:HB3  | 5        | 0.13          |
| (1,608) | 1:26:A:THR:HG22 | 1:27:A:SER:HB2  | 5        | 0.13          |
| (1,608) | 1:26:A:THR:HG22 | 1:27:A:SER:HB3  | 5        | 0.13          |
| (1,608) | 1:26:A:THR:HG23 | 1:27:A:SER:HB2  | 5        | 0.13          |
| (1,608) | 1:26:A:THR:HG23 | 1:27:A:SER:HB3  | 5        | 0.13          |
| (1,589) | 1:19:A:GLN:HG2  | 1:20:A:TRP:H    | 2        | 0.13          |
| (1,589) | 1:19:A:GLN:HG3  | 1:20:A:TRP:H    | 2        | 0.13          |
| (1,574) | 1:15:A:CYS:H    | 1:15:A:CYS:HB2  | 9        | 0.13          |
| (1,574) | 1:15:A:CYS:H    | 1:15:A:CYS:HB3  | 9        | 0.13          |
| (1,531) | 1:30:A:CYS:H    | 1:55:A:ILE:HG21 | 4        | 0.13          |
| (1,531) | 1:30:A:CYS:H    | 1:55:A:ILE:HG22 | 4        | 0.13          |
| (1,531) | 1:30:A:CYS:H    | 1:55:A:ILE:HG23 | 4        | 0.13          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG21 | 10       | 0.13          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG22 | 10       | 0.13          |
| (1,480) | 1:80:A:ASN:H    | 1:81:A:THR:HG23 | 10       | 0.13          |
| (1,461) | 1:69:A:TYR:HD1  | 1:89:A:SER:HA   | 9        | 0.13          |
| (1,461) | 1:69:A:TYR:HD2  | 1:89:A:SER:HA   | 9        | 0.13          |
| (1,420) | 1:35:A:ARG:H    | 1:36:A:GLU:HA   | 8        | 0.13          |
| (1,394) | 1:90:A:LEU:HD21 | 1:99:A:CYS:HB3  | 1        | 0.13          |
| (1,394) | 1:90:A:LEU:HD22 | 1:99:A:CYS:HB3  | 1        | 0.13          |
| (1,394) | 1:90:A:LEU:HD23 | 1:99:A:CYS:HB3  | 1        | 0.13          |
| (1,375) | 1:68:A:LYS:H    | 1:90:A:LEU:HD11 | 1        | 0.13          |
| (1,375) | 1:68:A:LYS:H    | 1:90:A:LEU:HD12 | 1        | 0.13          |
| (1,375) | 1:68:A:LYS:H    | 1:90:A:LEU:HD13 | 1        | 0.13          |
| (1,330) | 1:96:A:ASN:HA   | 1:97:A:ALA:H    | 7        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,312) | 1:7:A:GLU:HA    | 1:8:A:LYS:H     | 4        | 0.13          |
| (1,312) | 1:7:A:GLU:HA    | 1:8:A:LYS:H     | 8        | 0.13          |
| (1,307) | 1:26:A:THR:HG21 | 1:27:A:SER:HB2  | 1        | 0.13          |
| (1,307) | 1:26:A:THR:HG22 | 1:27:A:SER:HB2  | 1        | 0.13          |
| (1,307) | 1:26:A:THR:HG23 | 1:27:A:SER:HB2  | 1        | 0.13          |
| (1,297) | 1:26:A:THR:HB   | 1:32:A:LEU:HA   | 5        | 0.13          |
| (1,292) | 1:50:A:THR:HB   | 1:51:A:GLN:H    | 10       | 0.13          |
| (1,291) | 1:85:A:THR:HB   | 1:86:A:ARG:H    | 6        | 0.13          |
| (1,277) | 1:31:A:GLY:H    | 1:55:A:ILE:HB   | 2        | 0.13          |
| (1,263) | 1:16:A:GLY:H    | 1:40:A:THR:H    | 7        | 0.13          |
| (1,254) | 1:15:A:CYS:HA   | 1:16:A:GLY:H    | 1        | 0.13          |
| (1,254) | 1:15:A:CYS:HA   | 1:16:A:GLY:H    | 5        | 0.13          |
| (1,172) | 1:54:A:LYS:H    | 1:54:A:LYS:HG3  | 9        | 0.13          |
| (1,167) | 1:97:A:ALA:HB1  | 1:98:A:GLU:H    | 10       | 0.13          |
| (1,167) | 1:97:A:ALA:HB2  | 1:98:A:GLU:H    | 10       | 0.13          |
| (1,167) | 1:97:A:ALA:HB3  | 1:98:A:GLU:H    | 10       | 0.13          |
| (1,138) | 1:35:A:ARG:H    | 1:53:A:CYS:H    | 4        | 0.13          |
| (1,133) | 1:90:A:LEU:HG   | 1:99:A:CYS:H    | 4        | 0.13          |
| (1,109) | 1:8:A:LYS:H     | 1:8:A:LYS:HA    | 2        | 0.13          |
| (1,108) | 1:126:A:LYS:H   | 1:126:A:LYS:HA  | 3        | 0.13          |
| (1,102) | 1:18:A:TRP:HH2  | 1:48:A:MET:H    | 4        | 0.13          |
| (1,55)  | 1:18:A:TRP:H    | 1:18:A:TRP:HE3  | 9        | 0.13          |
| (1,1)   | 1:78:A:ASP:H    | 1:85:A:THR:H    | 4        | 0.13          |
| (1,820) | 1:126:A:LYS:HB2 | 1:127:A:GLU:H   | 2        | 0.12          |
| (1,820) | 1:126:A:LYS:HB3 | 1:127:A:GLU:H   | 2        | 0.12          |
| (1,817) | 1:120:A:GLU:H   | 1:120:A:GLU:HG2 | 6        | 0.12          |
| (1,817) | 1:120:A:GLU:H   | 1:120:A:GLU:HG3 | 6        | 0.12          |
| (1,810) | 1:113:A:THR:HA  | 1:115:A:PRO:HD2 | 7        | 0.12          |
| (1,810) | 1:113:A:THR:HA  | 1:115:A:PRO:HD3 | 7        | 0.12          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD11 | 5        | 0.12          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD12 | 5        | 0.12          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD13 | 5        | 0.12          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD21 | 5        | 0.12          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD22 | 5        | 0.12          |
| (1,768) | 1:92:A:ARG:HD2  | 1:94:A:LEU:HD23 | 5        | 0.12          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD11 | 5        | 0.12          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD12 | 5        | 0.12          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD13 | 5        | 0.12          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD21 | 5        | 0.12          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD22 | 5        | 0.12          |
| (1,768) | 1:92:A:ARG:HD3  | 1:94:A:LEU:HD23 | 5        | 0.12          |
| (1,763) | 1:92:A:ARG:HA   | 1:92:A:ARG:HD2  | 1        | 0.12          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,763) | 1:92:A:ARG:HA    | 1:92:A:ARG:HD3  | 1        | 0.12          |
| (1,746) | 1:83:A:LEU:HD11  | 1:108:A:PRO:HB2 | 4        | 0.12          |
| (1,746) | 1:83:A:LEU:HD11  | 1:108:A:PRO:HB3 | 4        | 0.12          |
| (1,746) | 1:83:A:LEU:HD12  | 1:108:A:PRO:HB2 | 4        | 0.12          |
| (1,746) | 1:83:A:LEU:HD12  | 1:108:A:PRO:HB3 | 4        | 0.12          |
| (1,746) | 1:83:A:LEU:HD13  | 1:108:A:PRO:HB2 | 4        | 0.12          |
| (1,746) | 1:83:A:LEU:HD13  | 1:108:A:PRO:HB3 | 4        | 0.12          |
| (1,722) | 1:72:A:GLN:HB2   | 1:87:A:THR:H    | 7        | 0.12          |
| (1,722) | 1:72:A:GLN:HB3   | 1:87:A:THR:H    | 7        | 0.12          |
| (1,708) | 1:68:A:LYS:H     | 1:68:A:LYS:HG2  | 8        | 0.12          |
| (1,708) | 1:68:A:LYS:H     | 1:68:A:LYS:HG3  | 8        | 0.12          |
| (1,688) | 1:61:A:LYS:HG2   | 1:62:A:GLN:H    | 10       | 0.12          |
| (1,688) | 1:61:A:LYS:HG3   | 1:62:A:GLN:H    | 10       | 0.12          |
| (1,572) | 1:13:A:SER:HB2   | 1:14:A:ASP:H    | 1        | 0.12          |
| (1,572) | 1:13:A:SER:HB3   | 1:14:A:ASP:H    | 1        | 0.12          |
| (1,571) | 1:13:A:SER:HA    | 1:14:A:ASP:HB2  | 8        | 0.12          |
| (1,571) | 1:13:A:SER:HA    | 1:14:A:ASP:HB3  | 8        | 0.12          |
| (1,447) | 1:69:A:TYR:HE1   | 1:89:A:SER:HA   | 7        | 0.12          |
| (1,447) | 1:69:A:TYR:HE2   | 1:89:A:SER:HA   | 7        | 0.12          |
| (1,366) | 1:83:A:LEU:HD11  | 1:109:A:CYS:H   | 3        | 0.12          |
| (1,366) | 1:83:A:LEU:HD12  | 1:109:A:CYS:H   | 3        | 0.12          |
| (1,366) | 1:83:A:LEU:HD13  | 1:109:A:CYS:H   | 3        | 0.12          |
| (1,283) | 1:81:A:THR:H     | 1:82:A:ALA:HA   | 4        | 0.12          |
| (1,283) | 1:81:A:THR:H     | 1:82:A:ALA:HA   | 9        | 0.12          |
| (1,275) | 1:63:A:PHE:HB3   | 1:64:A:GLY:H    | 10       | 0.12          |
| (1,254) | 1:15:A:CYS:HA    | 1:16:A:GLY:H    | 4        | 0.12          |
| (1,240) | 1:112:A:LEU:HD21 | 1:113:A:THR:H   | 3        | 0.12          |
| (1,240) | 1:112:A:LEU:HD22 | 1:113:A:THR:H   | 3        | 0.12          |
| (1,240) | 1:112:A:LEU:HD23 | 1:113:A:THR:H   | 3        | 0.12          |
| (1,237) | 1:76:A:GLU:H     | 1:76:A:GLU:HB2  | 8        | 0.12          |
| (1,231) | 1:80:A:ASN:H     | 1:80:A:ASN:HB3  | 9        | 0.12          |
| (1,204) | 1:105:A:ILE:HB   | 1:106:A:SER:H   | 8        | 0.12          |
| (1,193) | 1:50:A:THR:H     | 1:50:A:THR:HB   | 7        | 0.12          |
| (1,193) | 1:50:A:THR:H     | 1:50:A:THR:HB   | 9        | 0.12          |
| (1,172) | 1:54:A:LYS:H     | 1:54:A:LYS:HG3  | 7        | 0.12          |
| (1,167) | 1:97:A:ALA:HB1   | 1:98:A:GLU:H    | 3        | 0.12          |
| (1,167) | 1:97:A:ALA:HB2   | 1:98:A:GLU:H    | 3        | 0.12          |
| (1,167) | 1:97:A:ALA:HB3   | 1:98:A:GLU:H    | 3        | 0.12          |
| (1,146) | 1:27:A:SER:HA    | 1:29:A:ASP:H    | 1        | 0.12          |
| (1,109) | 1:8:A:LYS:H      | 1:8:A:LYS:HA    | 1        | 0.12          |
| (1,108) | 1:126:A:LYS:H    | 1:126:A:LYS:HA  | 1        | 0.12          |
| (1,108) | 1:126:A:LYS:H    | 1:126:A:LYS:HA  | 2        | 0.12          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,98)  | 1:60:A:LYS:H     | 1:61:A:LYS:H    | 7        | 0.12          |
| (1,69)  | 1:9:A:LYS:HA     | 1:10:A:VAL:H    | 4        | 0.12          |
| (1,55)  | 1:18:A:TRP:H     | 1:18:A:TRP:HE3  | 7        | 0.12          |
| (1,43)  | 1:90:A:LEU:HB3   | 1:101:A:LYS:H   | 5        | 0.12          |
| (1,40)  | 1:113:A:THR:HB   | 1:114:A:LYS:H   | 4        | 0.12          |
| (1,40)  | 1:113:A:THR:HB   | 1:114:A:LYS:H   | 8        | 0.12          |
| (1,816) | 1:120:A:GLU:H    | 1:120:A:GLU:HB2 | 9        | 0.11          |
| (1,816) | 1:120:A:GLU:H    | 1:120:A:GLU:HB3 | 9        | 0.11          |
| (1,766) | 1:92:A:ARG:HG2   | 1:93:A:ALA:H    | 6        | 0.11          |
| (1,766) | 1:92:A:ARG:HG3   | 1:93:A:ALA:H    | 6        | 0.11          |
| (1,716) | 1:70:A:GLN:HB2   | 1:89:A:SER:H    | 4        | 0.11          |
| (1,716) | 1:70:A:GLN:HB3   | 1:89:A:SER:H    | 4        | 0.11          |
| (1,681) | 1:60:A:LYS:HA    | 1:60:A:LYS:HD2  | 10       | 0.11          |
| (1,681) | 1:60:A:LYS:HA    | 1:60:A:LYS:HD3  | 10       | 0.11          |
| (1,670) | 1:54:A:LYS:H     | 1:54:A:LYS:HG2  | 5        | 0.11          |
| (1,670) | 1:54:A:LYS:H     | 1:54:A:LYS:HG3  | 5        | 0.11          |
| (1,639) | 1:43:A:GLU:HA    | 1:43:A:GLU:HG2  | 1        | 0.11          |
| (1,639) | 1:43:A:GLU:HA    | 1:43:A:GLU:HG3  | 1        | 0.11          |
| (1,636) | 1:42:A:ALA:HB1   | 1:43:A:GLU:HG2  | 1        | 0.11          |
| (1,636) | 1:42:A:ALA:HB1   | 1:43:A:GLU:HG3  | 1        | 0.11          |
| (1,636) | 1:42:A:ALA:HB2   | 1:43:A:GLU:HG2  | 1        | 0.11          |
| (1,636) | 1:42:A:ALA:HB2   | 1:43:A:GLU:HG3  | 1        | 0.11          |
| (1,636) | 1:42:A:ALA:HB3   | 1:43:A:GLU:HG2  | 1        | 0.11          |
| (1,636) | 1:42:A:ALA:HB3   | 1:43:A:GLU:HG3  | 1        | 0.11          |
| (1,613) | 1:28:A:GLY:HA2   | 1:30:A:CYS:H    | 10       | 0.11          |
| (1,613) | 1:28:A:GLY:HA3   | 1:30:A:CYS:H    | 10       | 0.11          |
| (1,478) | 1:104:A:THR:HG21 | 1:105:A:ILE:H   | 5        | 0.11          |
| (1,478) | 1:104:A:THR:HG22 | 1:105:A:ILE:H   | 5        | 0.11          |
| (1,478) | 1:104:A:THR:HG23 | 1:105:A:ILE:H   | 5        | 0.11          |
| (1,476) | 1:37:A:GLY:H     | 1:50:A:THR:HG21 | 5        | 0.11          |
| (1,476) | 1:37:A:GLY:H     | 1:50:A:THR:HG22 | 5        | 0.11          |
| (1,476) | 1:37:A:GLY:H     | 1:50:A:THR:HG23 | 5        | 0.11          |
| (1,468) | 1:115:A:PRO:HB3  | 1:117:A:PRO:HD3 | 6        | 0.11          |
| (1,377) | 1:18:A:TRP:HZ3   | 1:38:A:THR:HG21 | 4        | 0.11          |
| (1,377) | 1:18:A:TRP:HZ3   | 1:38:A:THR:HG22 | 4        | 0.11          |
| (1,377) | 1:18:A:TRP:HZ3   | 1:38:A:THR:HG23 | 4        | 0.11          |
| (1,366) | 1:83:A:LEU:HD11  | 1:109:A:CYS:H   | 2        | 0.11          |
| (1,366) | 1:83:A:LEU:HD12  | 1:109:A:CYS:H   | 2        | 0.11          |
| (1,366) | 1:83:A:LEU:HD13  | 1:109:A:CYS:H   | 2        | 0.11          |
| (1,351) | 1:90:A:LEU:HG    | 1:101:A:LYS:HA  | 1        | 0.11          |
| (1,332) | 1:39:A:ARG:HA    | 1:47:A:THR:HB   | 3        | 0.11          |
| (1,330) | 1:96:A:ASN:HA    | 1:97:A:ALA:H    | 2        | 0.11          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,316) | 1:89:A:SER:HA   | 1:90:A:LEU:HB3 | 1        | 0.11          |
| (1,316) | 1:89:A:SER:HA   | 1:90:A:LEU:HB3 | 8        | 0.11          |
| (1,316) | 1:89:A:SER:HA   | 1:90:A:LEU:HB3 | 9        | 0.11          |
| (1,286) | 1:79:A:LEU:HB2  | 1:81:A:THR:H   | 9        | 0.11          |
| (1,201) | 1:78:A:ASP:HB2  | 1:83:A:LEU:H   | 6        | 0.11          |
| (1,195) | 1:102:A:THR:HB  | 1:103:A:VAL:H  | 2        | 0.11          |
| (1,195) | 1:102:A:THR:HB  | 1:103:A:VAL:H  | 3        | 0.11          |
| (1,172) | 1:54:A:LYS:H    | 1:54:A:LYS:HG3 | 8        | 0.11          |
| (1,152) | 1:43:A:GLU:HA   | 1:44:A:CYS:H   | 10       | 0.11          |
| (1,134) | 1:90:A:LEU:HD21 | 1:99:A:CYS:H   | 2        | 0.11          |
| (1,134) | 1:90:A:LEU:HD22 | 1:99:A:CYS:H   | 2        | 0.11          |
| (1,134) | 1:90:A:LEU:HD23 | 1:99:A:CYS:H   | 2        | 0.11          |
| (1,133) | 1:90:A:LEU:HG   | 1:99:A:CYS:H   | 8        | 0.11          |
| (1,115) | 1:26:A:THR:H    | 1:27:A:SER:HB2 | 7        | 0.11          |
| (1,114) | 1:26:A:THR:H    | 1:27:A:SER:HB3 | 6        | 0.11          |
| (1,85)  | 1:85:A:THR:HG21 | 1:86:A:ARG:H   | 9        | 0.11          |
| (1,85)  | 1:85:A:THR:HG22 | 1:86:A:ARG:H   | 9        | 0.11          |
| (1,85)  | 1:85:A:THR:HG23 | 1:86:A:ARG:H   | 9        | 0.11          |
| (1,70)  | 1:104:A:THR:HB  | 1:105:A:ILE:H  | 8        | 0.11          |
| (1,67)  | 1:111:A:LYS:HA  | 1:112:A:LEU:H  | 8        | 0.11          |
| (1,40)  | 1:113:A:THR:HB  | 1:114:A:LYS:H  | 1        | 0.11          |
| (1,8)   | 1:69:A:TYR:HD1  | 1:90:A:LEU:H   | 10       | 0.11          |
| (1,8)   | 1:69:A:TYR:HD2  | 1:90:A:LEU:H   | 10       | 0.11          |
| (1,6)   | 1:77:A:CYS:HB2  | 1:78:A:ASP:H   | 3        | 0.11          |
| (1,661) | 1:51:A:GLN:HA   | 1:52:A:ARG:HD2 | 4        | 0.1           |
| (1,661) | 1:51:A:GLN:HA   | 1:52:A:ARG:HD3 | 4        | 0.1           |
| (1,660) | 1:51:A:GLN:HA   | 1:52:A:ARG:HG2 | 2        | 0.1           |
| (1,660) | 1:51:A:GLN:HA   | 1:52:A:ARG:HG3 | 2        | 0.1           |
| (1,449) | 1:69:A:TYR:HA   | 1:69:A:TYR:HE1 | 3        | 0.1           |
| (1,449) | 1:69:A:TYR:HA   | 1:69:A:TYR:HE2 | 3        | 0.1           |
| (1,448) | 1:18:A:TRP:HZ3  | 1:39:A:ARG:HA  | 10       | 0.1           |
| (1,438) | 1:18:A:TRP:HB3  | 1:18:A:TRP:HD1 | 2        | 0.1           |
| (1,342) | 1:54:A:LYS:HB3  | 1:55:A:ILE:H   | 4        | 0.1           |
| (1,323) | 1:26:A:THR:HG21 | 1:27:A:SER:HA  | 10       | 0.1           |
| (1,323) | 1:26:A:THR:HG22 | 1:27:A:SER:HA  | 10       | 0.1           |
| (1,323) | 1:26:A:THR:HG23 | 1:27:A:SER:HA  | 10       | 0.1           |
| (1,172) | 1:54:A:LYS:H    | 1:54:A:LYS:HG3 | 10       | 0.1           |
| (1,112) | 1:47:A:THR:HB   | 1:48:A:MET:H   | 7        | 0.1           |
| (1,108) | 1:126:A:LYS:H   | 1:126:A:LYS:HA | 10       | 0.1           |

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

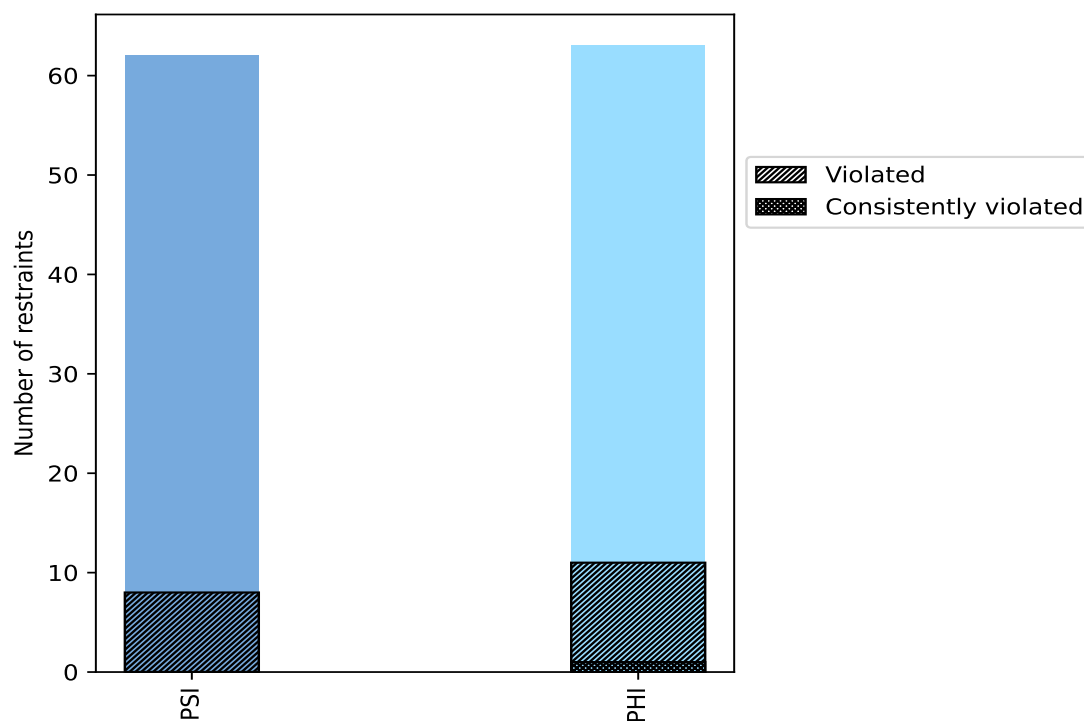
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 62    | 49.6           | 8                     | 12.9           | 6.4            | 0                                  | 0.0            | 0.0            |
| PHI        | 63    | 50.4           | 11                    | 17.5           | 8.8            | 1                                  | 1.6            | 0.8            |
| Total      | 125   | 100.0          | 19                    | 15.2           | 15.2           | 1                                  | 0.8            | 0.8            |

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

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



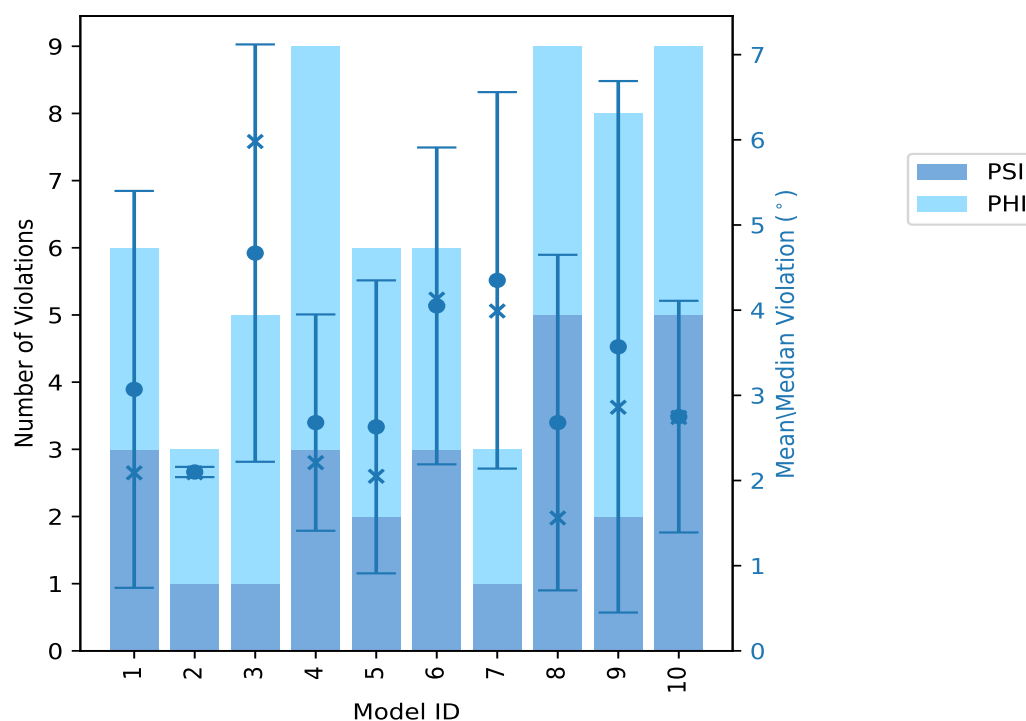
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model [i](#)

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 3                    | 3   | 6     | 3.07     | 8.21    | 2.33   | 2.09       |
| 2        | 1                    | 2   | 3     | 2.1      | 2.17    | 0.06   | 2.09       |
| 3        | 1                    | 4   | 5     | 4.67     | 7.3     | 2.45   | 5.98       |
| 4        | 3                    | 6   | 9     | 2.68     | 5.07    | 1.27   | 2.21       |
| 5        | 2                    | 4   | 6     | 2.63     | 6.24    | 1.72   | 2.05       |
| 6        | 3                    | 3   | 6     | 4.05     | 6.66    | 1.86   | 4.13       |
| 7        | 1                    | 2   | 3     | 4.35     | 7.22    | 2.21   | 3.99       |
| 8        | 5                    | 4   | 9     | 2.68     | 6.67    | 1.97   | 1.56       |
| 9        | 2                    | 6   | 8     | 3.57     | 11.37   | 3.12   | 2.86       |
| 10       | 5                    | 4   | 9     | 2.75     | 5.17    | 1.36   | 2.74       |

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



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

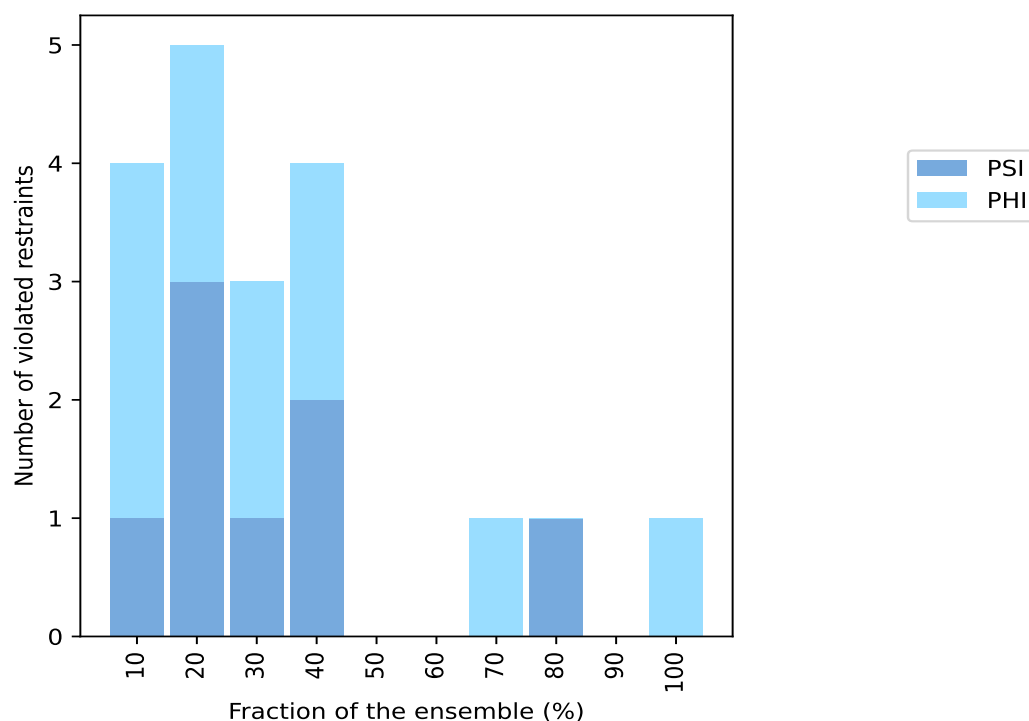
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 1                             | 3   | 4     | 1                        | 10.0  |
| 3                             | 2   | 5     | 2                        | 20.0  |
| 1                             | 2   | 3     | 3                        | 30.0  |
| 2                             | 2   | 4     | 4                        | 40.0  |
| 0                             | 0   | 0     | 5                        | 50.0  |
| 0                             | 0   | 0     | 6                        | 60.0  |
| 0                             | 1   | 1     | 7                        | 70.0  |
| 1                             | 0   | 1     | 8                        | 80.0  |
| 0                             | 0   | 0     | 9                        | 90.0  |
| 0                             | 1   | 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](#)

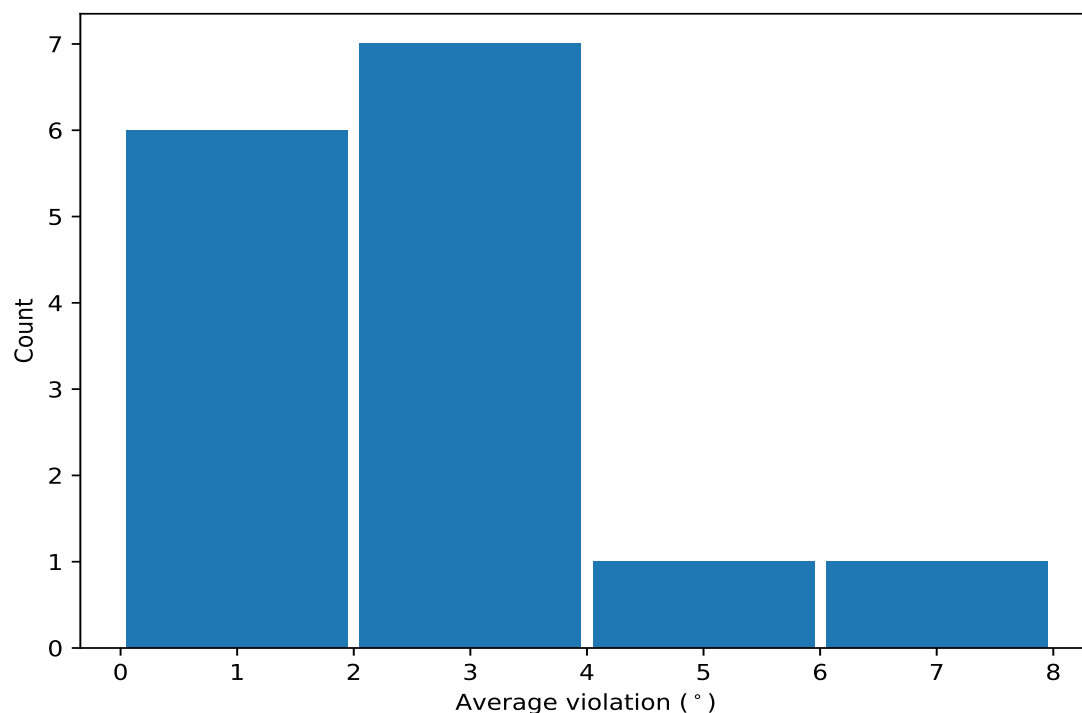




## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 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 |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,15)  | 1:21:A:SER:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 10                  | 6.02 | 2.4             | 5.86   |
| (1,6)   | 1:17:A:GLU:N | 1:17:A:GLU:CA | 1:17:A:GLU:C  | 1:18:A:TRP:N | 8                   | 4.51 | 1.85            | 4.56   |
| (1,7)   | 1:17:A:GLU:C | 1:18:A:TRP:N  | 1:18:A:TRP:CA | 1:18:A:TRP:C | 7                   | 3.35 | 1.62            | 3.33   |
| (1,22)  | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:GLY:N | 4                   | 3.1  | 2.41            | 1.98   |
| (1,5)   | 1:16:A:GLY:C | 1:17:A:GLU:N  | 1:17:A:GLU:CA | 1:17:A:GLU:C | 4                   | 2.38 | 0.87            | 2.26   |
| (1,4)   | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C  | 1:17:A:GLU:N | 4                   | 1.86 | 0.85            | 1.57   |
| (1,95)  | 1:88:A:GLY:C | 1:89:A:SER:N  | 1:89:A:SER:CA | 1:89:A:SER:C | 4                   | 1.52 | 0.3             | 1.49   |
| (1,102) | 1:92:A:ARG:C | 1:93:A:ALA:N  | 1:93:A:ALA:CA | 1:93:A:ALA:C | 3                   | 2.49 | 1.37            | 1.67   |
| (1,35)  | 1:39:A:ARG:C | 1:40:A:THR:N  | 1:40:A:THR:CA | 1:40:A:THR:C | 3                   | 2.09 | 0.2             | 2.03   |
| (1,105) | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C  | 1:95:A:HIS:N | 3                   | 1.82 | 0.13            | 1.74   |
| (1,2)   | 1:14:A:ASP:N | 1:14:A:ASP:CA | 1:14:A:ASP:C  | 1:15:A:CYS:N | 2                   | 2.92 | 0.21            | 2.92   |
| (1,14)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:VAL:N | 2                   | 2.8  | 0.12            | 2.8    |
| (1,19)  | 1:30:A:CYS:C | 1:31:A:GLY:N  | 1:31:A:GLY:CA | 1:31:A:GLY:C | 2                   | 1.9  | 0.74            | 1.9    |

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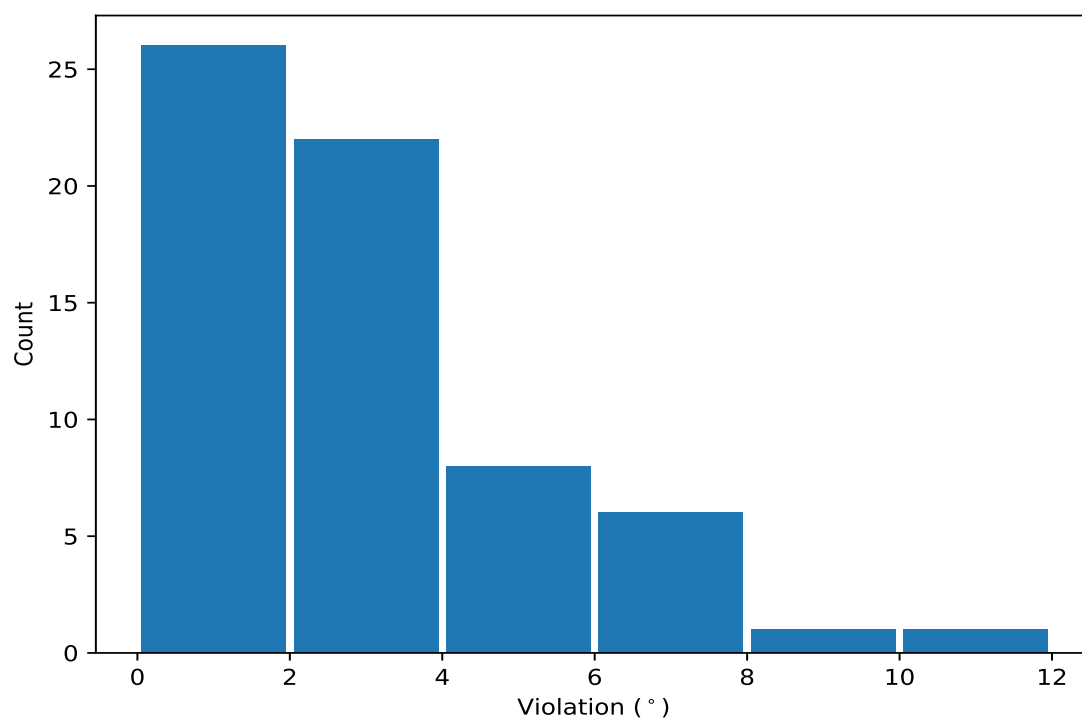
| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,21)  | 1:31:A:GLY:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C | 2                   | 1.43 | 0.41            | 1.43   |
| (1,109) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C  | 1:99:A:CYS:N | 2                   | 1.34 | 0.22            | 1.34   |

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

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

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

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



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

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

| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,15) | 1:21:A:SER:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 9        | 11.37         |
| (1,15) | 1:21:A:SER:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 1        | 8.21          |
| (1,6)  | 1:17:A:GLU:N | 1:17:A:GLU:CA | 1:17:A:GLU:C  | 1:18:A:TRP:N | 3        | 7.3           |
| (1,22) | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:GLY:N | 7        | 7.22          |
| (1,15) | 1:21:A:SER:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 8        | 6.67          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,6)   | 1:17:A:GLU:N | 1:17:A:GLU:CA | 1:17:A:GLU:C  | 1:18:A:TRP:N | 6        | 6.66          |
| (1,15)  | 1:21:A:SER:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 3        | 6.65          |
| (1,15)  | 1:21:A:SER:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 5        | 6.24          |
| (1,7)   | 1:17:A:GLU:C | 1:18:A:TRP:N  | 1:18:A:TRP:CA | 1:18:A:TRP:C | 3        | 5.98          |
| (1,6)   | 1:17:A:GLU:N | 1:17:A:GLU:CA | 1:17:A:GLU:C  | 1:18:A:TRP:N | 8        | 5.66          |
| (1,15)  | 1:21:A:SER:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 6        | 5.47          |
| (1,6)   | 1:17:A:GLU:N | 1:17:A:GLU:CA | 1:17:A:GLU:C  | 1:18:A:TRP:N | 10       | 5.17          |
| (1,7)   | 1:17:A:GLU:C | 1:18:A:TRP:N  | 1:18:A:TRP:CA | 1:18:A:TRP:C | 6        | 5.13          |
| (1,15)  | 1:21:A:SER:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 4        | 5.07          |
| (1,102) | 1:92:A:ARG:C | 1:93:A:ALA:N  | 1:93:A:ALA:CA | 1:93:A:ALA:C | 4        | 4.42          |
| (1,15)  | 1:21:A:SER:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 10       | 4.4           |
| (1,15)  | 1:21:A:SER:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 7        | 3.99          |
| (1,6)   | 1:17:A:GLU:N | 1:17:A:GLU:CA | 1:17:A:GLU:C  | 1:18:A:TRP:N | 9        | 3.95          |
| (1,7)   | 1:17:A:GLU:C | 1:18:A:TRP:N  | 1:18:A:TRP:CA | 1:18:A:TRP:C | 10       | 3.63          |
| (1,5)   | 1:16:A:GLY:C | 1:17:A:GLU:N  | 1:17:A:GLU:CA | 1:17:A:GLU:C | 9        | 3.63          |
| (1,3)   | 1:15:A:CYS:C | 1:16:A:GLY:N  | 1:16:A:GLY:CA | 1:16:A:GLY:C | 4        | 3.34          |
| (1,7)   | 1:17:A:GLU:C | 1:18:A:TRP:N  | 1:18:A:TRP:CA | 1:18:A:TRP:C | 8        | 3.33          |
| (1,4)   | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C  | 1:17:A:GLU:N | 9        | 3.22          |
| (1,2)   | 1:14:A:ASP:N | 1:14:A:ASP:CA | 1:14:A:ASP:C  | 1:15:A:CYS:N | 6        | 3.13          |
| (1,14)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:VAL:N | 10       | 2.93          |
| (1,6)   | 1:17:A:GLU:N | 1:17:A:GLU:CA | 1:17:A:GLU:C  | 1:18:A:TRP:N | 5        | 2.92          |
| (1,5)   | 1:16:A:GLY:C | 1:17:A:GLU:N  | 1:17:A:GLU:CA | 1:17:A:GLU:C | 10       | 2.74          |
| (1,2)   | 1:14:A:ASP:N | 1:14:A:ASP:CA | 1:14:A:ASP:C  | 1:15:A:CYS:N | 1        | 2.71          |
| (1,14)  | 1:21:A:SER:N | 1:21:A:SER:CA | 1:21:A:SER:C  | 1:22:A:VAL:N | 6        | 2.68          |
| (1,19)  | 1:30:A:CYS:C | 1:31:A:GLY:N  | 1:31:A:GLY:CA | 1:31:A:GLY:C | 4        | 2.64          |
| (1,7)   | 1:17:A:GLU:C | 1:18:A:TRP:N  | 1:18:A:TRP:CA | 1:18:A:TRP:C | 9        | 2.5           |
| (1,35)  | 1:39:A:ARG:C | 1:40:A:THR:N  | 1:40:A:THR:CA | 1:40:A:THR:C | 5        | 2.35          |
| (1,6)   | 1:17:A:GLU:N | 1:17:A:GLU:CA | 1:17:A:GLU:C  | 1:18:A:TRP:N | 1        | 2.27          |
| (1,22)  | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:GLY:N | 4        | 2.21          |
| (1,6)   | 1:17:A:GLU:N | 1:17:A:GLU:CA | 1:17:A:GLU:C  | 1:18:A:TRP:N | 2        | 2.17          |
| (1,15)  | 1:21:A:SER:C | 1:22:A:VAL:N  | 1:22:A:VAL:CA | 1:22:A:VAL:C | 2        | 2.09          |
| (1,35)  | 1:39:A:ARG:C | 1:40:A:THR:N  | 1:40:A:THR:CA | 1:40:A:THR:C | 2        | 2.03          |
| (1,105) | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C  | 1:95:A:HIS:N | 10       | 2.01          |
| (1,4)   | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C  | 1:17:A:GLU:N | 4        | 1.92          |
| (1,95)  | 1:88:A:GLY:C | 1:89:A:SER:N  | 1:89:A:SER:CA | 1:89:A:SER:C | 1        | 1.91          |
| (1,35)  | 1:39:A:ARG:C | 1:40:A:THR:N  | 1:40:A:THR:CA | 1:40:A:THR:C | 4        | 1.88          |
| (1,21)  | 1:31:A:GLY:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C | 7        | 1.84          |
| (1,5)   | 1:16:A:GLY:C | 1:17:A:GLU:N  | 1:17:A:GLU:CA | 1:17:A:GLU:C | 3        | 1.77          |
| (1,22)  | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:GLY:N | 5        | 1.75          |
| (1,105) | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C  | 1:95:A:HIS:N | 1        | 1.74          |
| (1,105) | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C  | 1:95:A:HIS:N | 8        | 1.72          |
| (1,95)  | 1:88:A:GLY:C | 1:89:A:SER:N  | 1:89:A:SER:CA | 1:89:A:SER:C | 9        | 1.72          |
| (1,102) | 1:92:A:ARG:C | 1:93:A:ALA:N  | 1:93:A:ALA:CA | 1:93:A:ALA:C | 3        | 1.67          |
| (1,67)  | 1:71:A:PHE:C | 1:72:A:GLN:N  | 1:72:A:GLN:CA | 1:72:A:GLN:C | 10       | 1.63          |
| (1,7)   | 1:17:A:GLU:C | 1:18:A:TRP:N  | 1:18:A:TRP:CA | 1:18:A:TRP:C | 1        | 1.58          |
| (1,109) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C  | 1:99:A:CYS:N | 8        | 1.56          |
| (1,83)  | 1:82:A:ALA:C | 1:83:A:LEU:N  | 1:83:A:LEU:CA | 1:83:A:LEU:C | 4        | 1.49          |
| (1,5)   | 1:16:A:GLY:C | 1:17:A:GLU:N  | 1:17:A:GLU:CA | 1:17:A:GLU:C | 8        | 1.4           |
| (1,102) | 1:92:A:ARG:C | 1:93:A:ALA:N  | 1:93:A:ALA:CA | 1:93:A:ALA:C | 8        | 1.38          |
| (1,7)   | 1:17:A:GLU:C | 1:18:A:TRP:N  | 1:18:A:TRP:CA | 1:18:A:TRP:C | 5        | 1.27          |
| (1,95)  | 1:88:A:GLY:C | 1:89:A:SER:N  | 1:89:A:SER:CA | 1:89:A:SER:C | 5        | 1.26          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,4)   | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C  | 1:17:A:GLU:N | 8        | 1.22          |
| (1,95)  | 1:88:A:GLY:C | 1:89:A:SER:N  | 1:89:A:SER:CA | 1:89:A:SER:C | 6        | 1.21          |
| (1,22)  | 1:32:A:LEU:N | 1:32:A:LEU:CA | 1:32:A:LEU:C  | 1:33:A:GLY:N | 8        | 1.2           |
| (1,19)  | 1:30:A:CYS:C | 1:31:A:GLY:N  | 1:31:A:GLY:CA | 1:31:A:GLY:C | 9        | 1.16          |
| (1,109) | 1:98:A:GLU:N | 1:98:A:GLU:CA | 1:98:A:GLU:C  | 1:99:A:CYS:N | 10       | 1.13          |
| (1,66)  | 1:71:A:PHE:N | 1:71:A:PHE:CA | 1:71:A:PHE:C  | 1:72:A:GLN:N | 4        | 1.12          |
| (1,4)   | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C  | 1:17:A:GLU:N | 10       | 1.07          |
| (1,21)  | 1:31:A:GLY:C | 1:32:A:LEU:N  | 1:32:A:LEU:CA | 1:32:A:LEU:C | 9        | 1.02          |