



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 01:33 AM UTC

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BMRB ID : 34033  
Title : Engineering protein stability with atomic precision in a monomeric miniprotein  
Authors : Baker, E.G.; Williams, C.; Hudson, K.L.; Bartlett, G.G.; Heal, J.W.; Sessions, R.B.; Crump, M.P.; Woolfson, D.N.  
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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
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

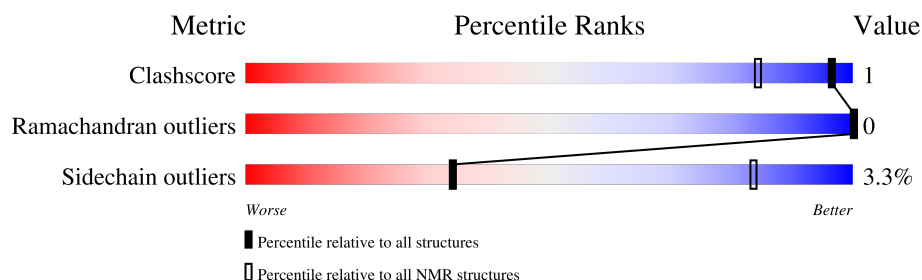
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 61%.

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     | 36     |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues |                                     |                   |              |
|--------------------------------------|-------------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)               | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:2-A:19, A:21-A:26, A:28-A:33 (30) | 0.46              | 17           |

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

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

The models can be grouped into 3 clusters and 6 single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 547 atoms, of which 277 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PPa-CH3.

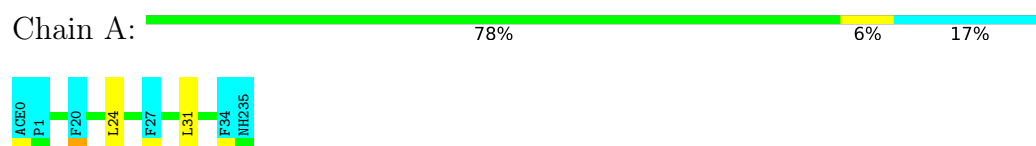
| Mol | Chain | Residues | Atoms |     |     |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|-------|
| 1   | A     | 36       | Total | C   | H   | N  | O  | 1     |
|     |       |          | 547   | 175 | 277 | 44 | 51 |       |

## 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: PPa-CH3

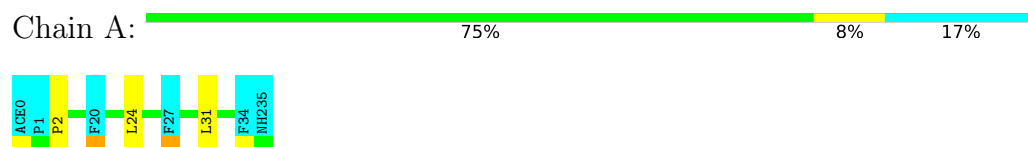


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

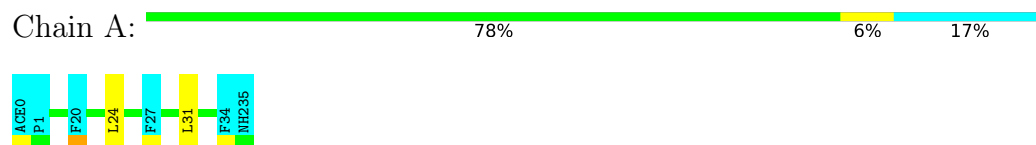
#### 4.2.1 Score per residue for model 1

- Molecule 1: PPa-CH3



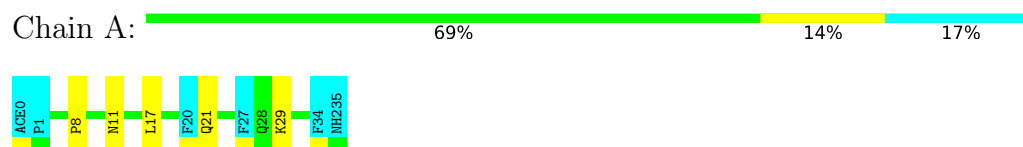
#### 4.2.2 Score per residue for model 2

- Molecule 1: PPa-CH3



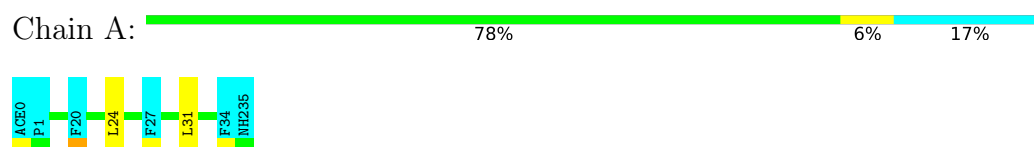
### 4.2.3 Score per residue for model 3

- Molecule 1: PPa-CH3



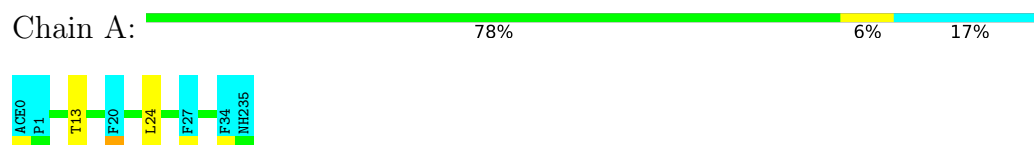
### 4.2.4 Score per residue for model 4

- Molecule 1: PPa-CH3



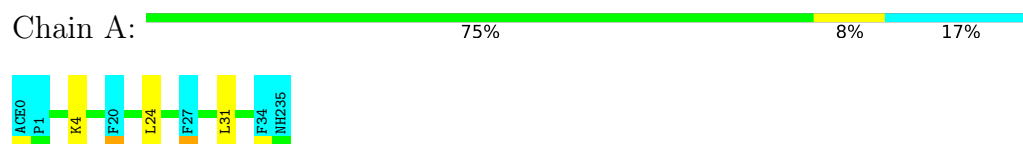
### 4.2.5 Score per residue for model 5

- Molecule 1: PPa-CH3



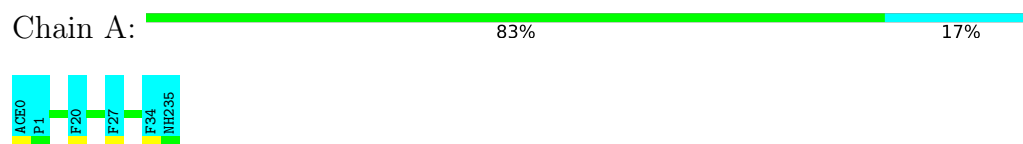
### 4.2.6 Score per residue for model 6

- Molecule 1: PPa-CH3



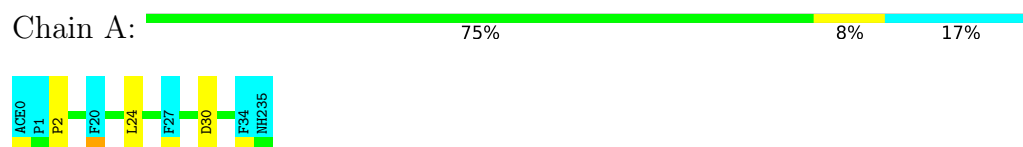
### 4.2.7 Score per residue for model 7

- Molecule 1: PPa-CH3



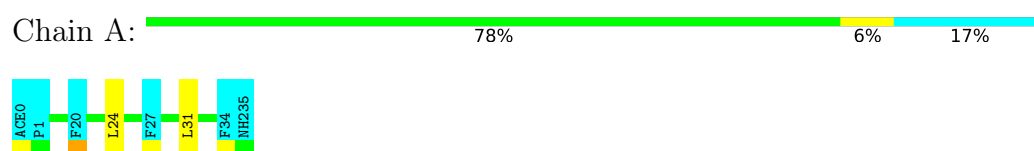
#### 4.2.8 Score per residue for model 8

- Molecule 1: PPa-CH3



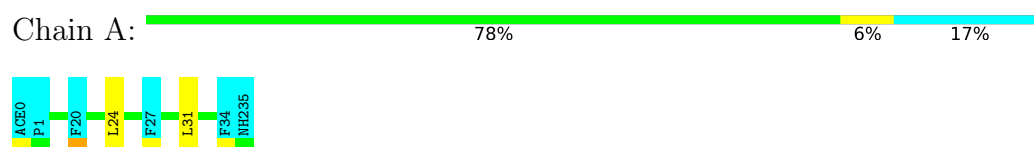
#### 4.2.9 Score per residue for model 9

- Molecule 1: PPa-CH3



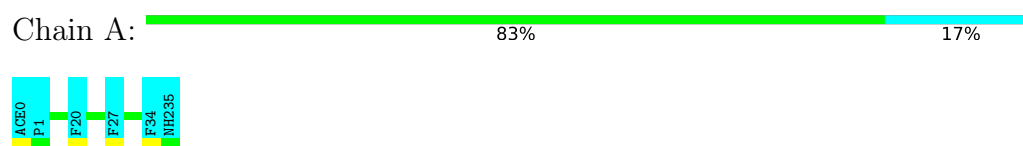
#### 4.2.10 Score per residue for model 10

- Molecule 1: PPa-CH3



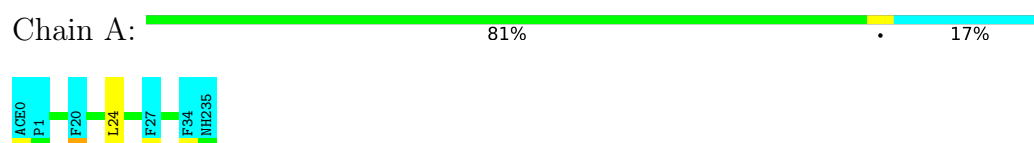
#### 4.2.11 Score per residue for model 11

- Molecule 1: PPa-CH3



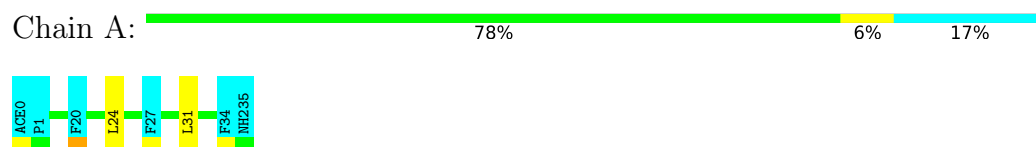
#### 4.2.12 Score per residue for model 12

- Molecule 1: PPa-CH3



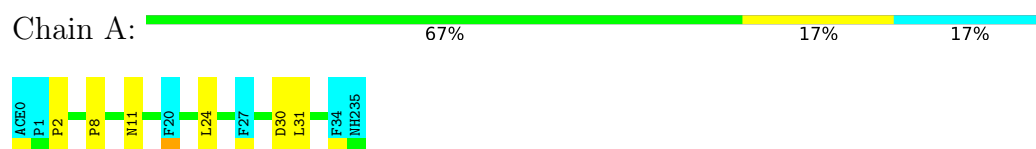
#### 4.2.13 Score per residue for model 13

- Molecule 1: PPa-CH3



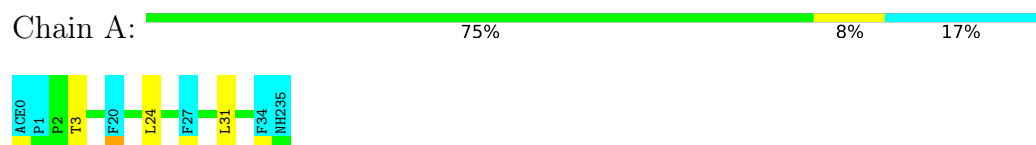
#### 4.2.14 Score per residue for model 14

- Molecule 1: PPa-CH3



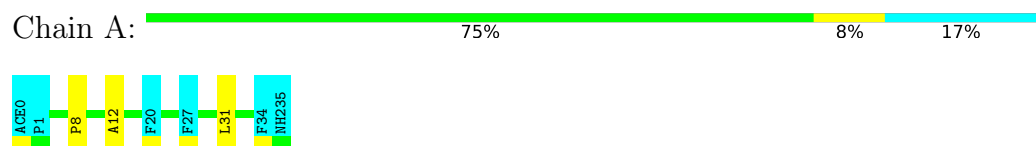
#### 4.2.15 Score per residue for model 15

- Molecule 1: PPa-CH3



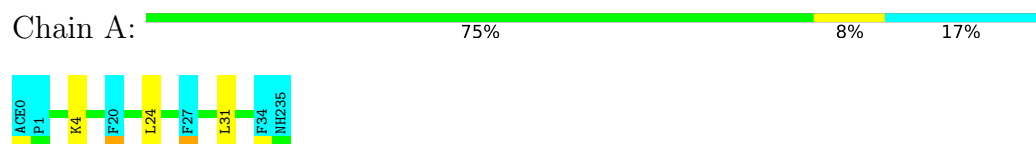
#### 4.2.16 Score per residue for model 16

- Molecule 1: PPa-CH3



#### 4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: PPa-CH3

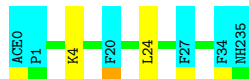




#### 4.2.18 Score per residue for model 18

- Molecule 1: PPa-CH3

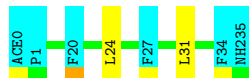
Chain A:  78% 6% 17%



#### 4.2.19 Score per residue for model 19

- Molecule 1: PPa-CH3

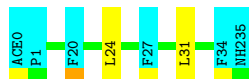
Chain A:  78% 6% 17%



#### 4.2.20 Score per residue for model 20

- Molecule 1: PPa-CH3

Chain A:  78% 6% 17%



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 20 were deposited, based on the following criterion: ?.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| ARIA          | refinement            | 2.3     |
| CNS           | structure calculation |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 297            |
| Number of shifts mapped to atoms             | 297            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 61%            |

## 6 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 4PH, NH2, ACE

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     | 223   | 232      | 232      | 0±1     |
| All | All   | 4460  | 4640     | 4640     | 7       |

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 1.

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

| Atom-1        | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|---------------|----------------|----------|-------------|--------|-------|
|               |                |          |             | Worst  | Total |
| 1:A:4:LYS:O   | 1:A:4:LYS:HD2  | 0.54     | 2.03        | 18     | 1     |
| 1:A:8:PRO:HB3 | 1:A:11:ASN:ND2 | 0.52     | 2.19        | 3      | 1     |
| 1:A:8:PRO:HA  | 1:A:11:ASN:OD1 | 0.42     | 2.15        | 14     | 1     |
| 1:A:17:LEU:O  | 1:A:21:GLN:HG2 | 0.41     | 2.15        | 3      | 1     |
| 1:A:2:PRO:HG3 | 1:A:30:ASP:OD2 | 0.41     | 2.15        | 8      | 1     |
| 1:A:8:PRO:O   | 1:A:12:ALA:HB2 | 0.41     | 2.16        | 16     | 1     |
| 1:A:2:PRO:HB3 | 1:A:30:ASP:OD2 | 0.41     | 2.16        | 14     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed      | Favoured     | Allowed    | Outliers   | Percentiles |     |
|-----|-------|---------------|--------------|------------|------------|-------------|-----|
| 1   | A     | 30/36 (83%)   | 27±1 (91±2%) | 3±1 (9±2%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 600/720 (83%) | 548 (91%)    | 52 (9%)    | 0 (0%)     | 100         | 100 |

There are no Ramachandran outliers.

### 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     | 24/25 (96%)   | 23±1 (97±2%) | 1±1 (3±2%) | 34          | 83 |
| All | All   | 480/500 (96%) | 464 (97%)    | 16 (3%)    | 34          | 83 |

All 4 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     | 31  | LEU  | 13             |
| 1   | A     | 29  | LYS  | 1              |
| 1   | A     | 13  | THR  | 1              |
| 1   | A     | 3   | THR  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths |           |            |
|-----|------|-------|-----|------|--------------|-----------|------------|
|     |      |       |     |      | Counts       | RMSZ      | #Z>2       |
| 1   | 4PH  | A     | 27  | 1    | 11,12,13     | 1.27±0.01 | 1±0 (9±0%) |
| 1   | 4PH  | A     | 34  | 1    | 11,12,13     | 1.27±0.02 | 1±0 (9±0%) |
| 1   | 4PH  | A     | 20  | 1    | 11,12,13     | 1.28±0.01 | 1±0 (9±0%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles |           |            |
|-----|------|-------|-----|------|-------------|-----------|------------|
|     |      |       |     |      | Counts      | RMSZ      | #Z>2       |
| 1   | 4PH  | A     | 27  | 1    | 10,15,17    | 0.78±0.02 | 0±0 (0±0%) |
| 1   | 4PH  | A     | 34  | 1    | 10,15,17    | 0.78±0.01 | 0±0 (0±0%) |
| 1   | 4PH  | A     | 20  | 1    | 10,15,17    | 0.78±0.02 | 0±0 (0±0%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings     |
|-----|------|-------|-----|------|---------|-----------|-----------|
| 1   | 4PH  | A     | 27  | 1    | -       | 0±0,5,6,8 | 0±0,1,1,1 |
| 1   | 4PH  | A     | 34  | 1    | -       | 0±0,5,6,8 | 0±0,1,1,1 |
| 1   | 4PH  | A     | 20  | 1    | -       | 0±0,5,6,8 | 0±0,1,1,1 |

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

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|--------|------|-------------|----------|--------|-------|
|     |       |     |      |        |      |             |          | Worst  | Total |
| 1   | A     | 20  | 4PH  | C33-CZ | 4.10 | 1.39        | 1.51     | 11     | 20    |
| 1   | A     | 27  | 4PH  | C33-CZ | 4.09 | 1.39        | 1.51     | 19     | 20    |
| 1   | A     | 34  | 4PH  | C33-CZ | 4.07 | 1.39        | 1.51     | 3      | 20    |

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 61% for the well-defined parts and 61% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *PaMe\_TMS\_converted.csdep*

#### 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                  | 297 |
| Number of shifts mapped to atoms        | 297 |
| 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           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 11       | —                               | None (insufficient data)   |
| $^{13}\text{C}_\beta$  | 5        | —                               | None (insufficient data)   |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 26       | $-0.17 \pm 0.38$                | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 61%, i.e. 233 atoms were assigned a chemical shift out of a possible 384. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 92/143 (64%)  | 56/57 (98%)   | 10/60 (17%)     | 26/26 (100%)    |
| Sidechain | 141/241 (59%) | 128/154 (83%) | 10/78 (13%)     | 3/9 (33%)       |

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|         | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|---------|---------------|----------------|-----------------|-----------------|
| Overall | 233/384 (61%) | 184/211 (87%)  | 20/138 (14%)    | 29/35 (83%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 61%, i.e. 241 atoms were assigned a chemical shift out of a possible 396. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 94/146 (64%)  | 57/58 (98%)    | 11/62 (18%)     | 26/26 (100%)    |
| Sidechain | 147/250 (59%) | 134/160 (84%)  | 10/81 (12%)     | 3/9 (33%)       |
| Overall   | 241/396 (61%) | 191/218 (88%)  | 21/143 (15%)    | 29/35 (83%)     |

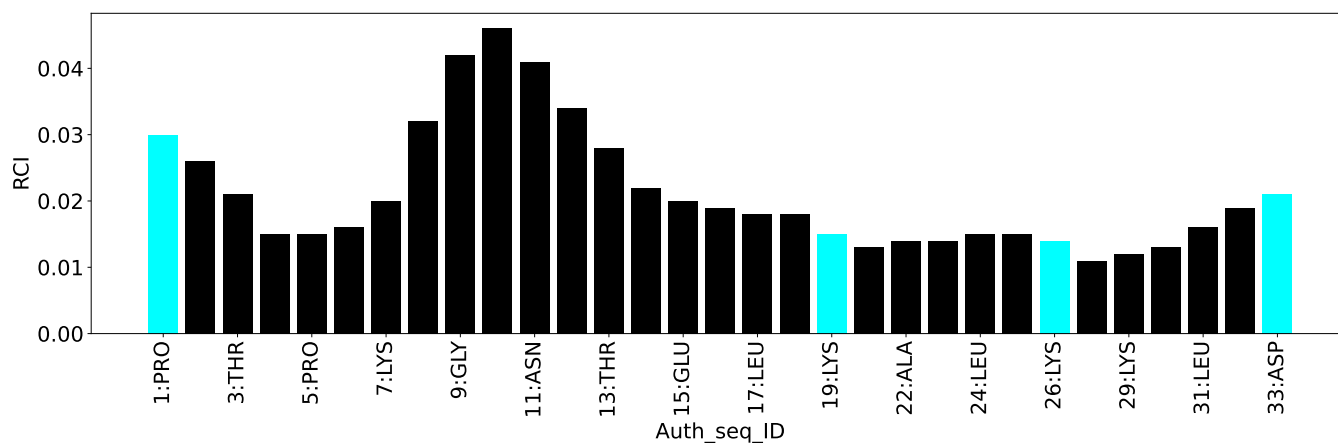
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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                                | 489   |
| Intra-residue ( $ i-j =0$ )                              | 256   |
| Sequential ( $ i-j =1$ )                                 | 116   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 66    |
| Long range ( $ i-j \geq 5$ )                             | 51    |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 48    |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 14.9  |
| Number of long range restraints per residue <sup>1</sup> | 1.4   |

<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)  | 8.8                                    | 0.2     |
| 0.2-0.5 (Medium) | 24.9                                   | 0.5     |
| >0.5 (Large)     | 36.8                                   | 5.98    |

### 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)   | 2.1                                    | 3.38    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

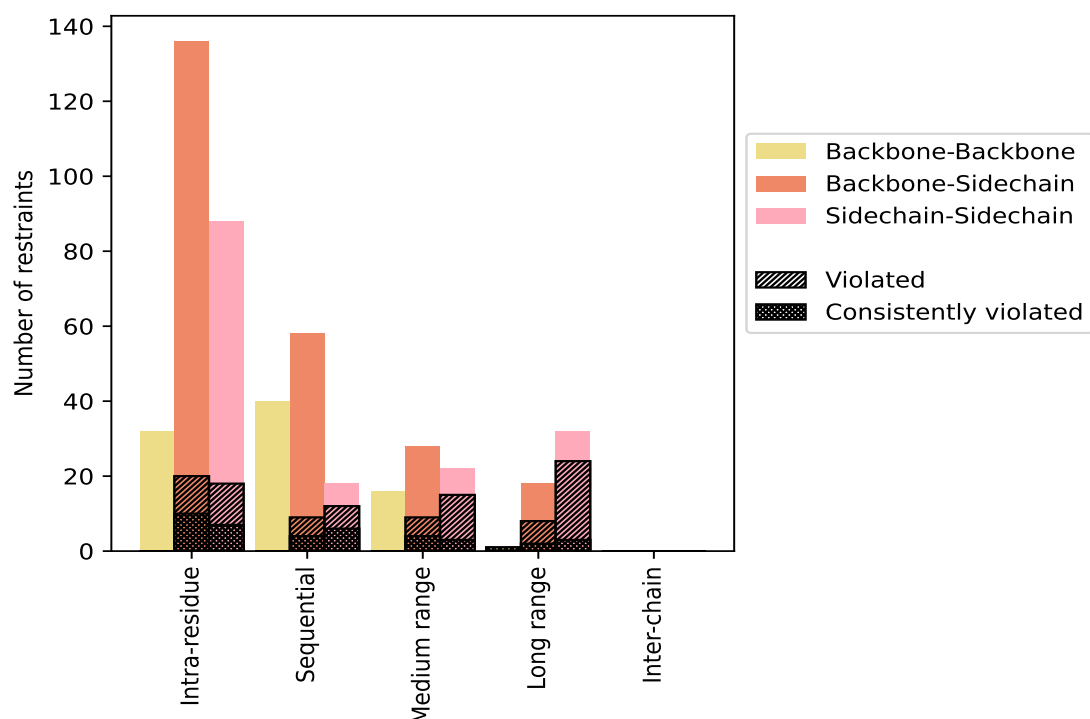
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count      | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |            |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>256</b> | <b>52.4</b>    | <b>38</b>             | <b>14.8</b>    | <b>7.8</b>     | <b>17</b>                          | <b>6.6</b>     | <b>3.5</b>     |
| Backbone-Backbone                                                           | 32         | 6.5            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 136        | 27.8           | 20                    | 14.7           | 4.1            | 10                                 | 7.4            | 2.0            |
| Sidechain-Sidechain                                                         | 88         | 18.0           | 18                    | 20.5           | 3.7            | 7                                  | 8.0            | 1.4            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>116</b> | <b>23.7</b>    | <b>21</b>             | <b>18.1</b>    | <b>4.3</b>     | <b>10</b>                          | <b>8.6</b>     | <b>2.0</b>     |
| Backbone-Backbone                                                           | 40         | 8.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 58         | 11.9           | 9                     | 15.5           | 1.8            | 4                                  | 6.9            | 0.8            |
| Sidechain-Sidechain                                                         | 18         | 3.7            | 12                    | 66.7           | 2.5            | 6                                  | 33.3           | 1.2            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>66</b>  | <b>13.5</b>    | <b>24</b>             | <b>36.4</b>    | <b>4.9</b>     | <b>7</b>                           | <b>10.6</b>    | <b>1.4</b>     |
| Backbone-Backbone                                                           | 16         | 3.3            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 28         | 5.7            | 9                     | 32.1           | 1.8            | 4                                  | 14.3           | 0.8            |
| Sidechain-Sidechain                                                         | 22         | 4.5            | 15                    | 68.2           | 3.1            | 3                                  | 13.6           | 0.6            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>51</b>  | <b>10.4</b>    | <b>33</b>             | <b>64.7</b>    | <b>6.7</b>     | <b>6</b>                           | <b>11.8</b>    | <b>1.2</b>     |
| Backbone-Backbone                                                           | 1          | 0.2            | 1                     | 100.0          | 0.2            | 1                                  | 100.0          | 0.2            |
| Backbone-Sidechain                                                          | 18         | 3.7            | 8                     | 44.4           | 1.6            | 2                                  | 11.1           | 0.4            |
| Sidechain-Sidechain                                                         | 32         | 6.5            | 24                    | 75.0           | 4.9            | 3                                  | 9.4            | 0.6            |
| <b>Inter-chain</b>                                                          | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>489</b> | <b>100.0</b>   | <b>116</b>            | <b>23.7</b>    | <b>23.7</b>    | <b>40</b>                          | <b>8.2</b>     | <b>8.2</b>     |
| Backbone-Backbone                                                           | 89         | 18.2           | 1                     | 1.1            | 0.2            | 1                                  | 1.1            | 0.2            |
| Backbone-Sidechain                                                          | 240        | 49.1           | 46                    | 19.2           | 9.4            | 20                                 | 8.3            | 4.1            |
| Sidechain-Sidechain                                                         | 160        | 32.7           | 69                    | 43.1           | 14.1           | 19                                 | 11.9           | 3.9            |

<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        | 28                   | 17              | 9               | 16              | 0               | 70    | 0.75     | 3.59    | 0.7                 | 0.52       |
| 2        | 31                   | 17              | 10              | 18              | 0               | 76    | 0.82     | 4.96    | 0.81                | 0.58       |
| 3        | 28                   | 18              | 12              | 20              | 0               | 78    | 0.79     | 4.97    | 0.81                | 0.58       |
| 4        | 27                   | 16              | 9               | 13              | 0               | 65    | 0.83     | 4.35    | 0.81                | 0.52       |
| 5        | 29                   | 17              | 11              | 13              | 0               | 70    | 0.78     | 3.47    | 0.74                | 0.52       |
| 6        | 25                   | 16              | 10              | 15              | 0               | 66    | 0.76     | 5.08    | 0.8                 | 0.52       |
| 7        | 26                   | 17              | 10              | 12              | 0               | 65    | 0.81     | 3.63    | 0.79                | 0.5        |
| 8        | 26                   | 14              | 11              | 13              | 0               | 64    | 0.78     | 3.54    | 0.71                | 0.55       |
| 9        | 27                   | 15              | 9               | 16              | 0               | 67    | 0.75     | 5.01    | 0.79                | 0.58       |
| 10       | 27                   | 16              | 11              | 17              | 0               | 71    | 0.79     | 4.0     | 0.77                | 0.49       |

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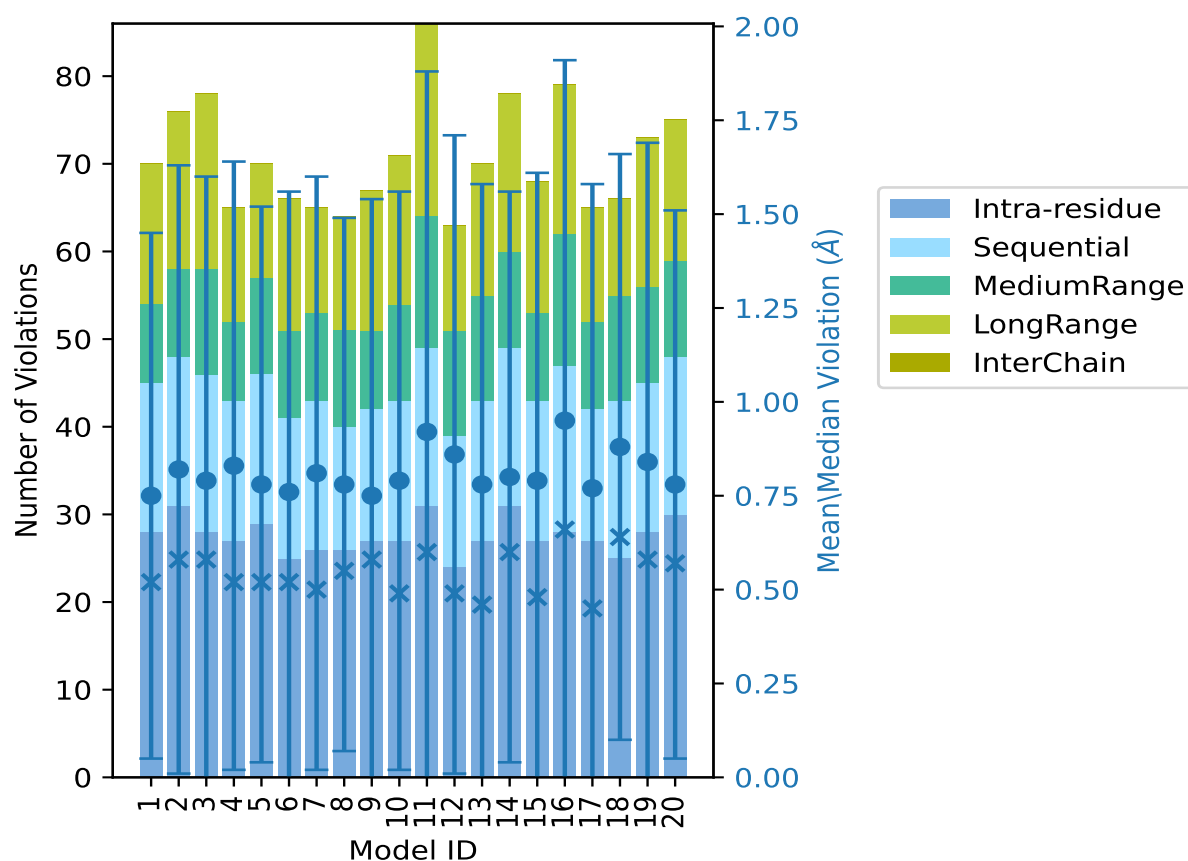
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 31                   | 18              | 15              | 22              | 0               | 86    | 0.92     | 5.91    | 0.96                | 0.6        |
| 12       | 24                   | 15              | 12              | 12              | 0               | 63    | 0.86     | 4.07    | 0.85                | 0.49       |
| 13       | 27                   | 16              | 12              | 15              | 0               | 70    | 0.78     | 4.84    | 0.8                 | 0.46       |
| 14       | 31                   | 18              | 11              | 18              | 0               | 78    | 0.8      | 4.67    | 0.76                | 0.6        |
| 15       | 27                   | 16              | 10              | 15              | 0               | 68    | 0.79     | 4.29    | 0.82                | 0.48       |
| 16       | 28                   | 19              | 15              | 17              | 0               | 79    | 0.95     | 5.98    | 0.96                | 0.66       |
| 17       | 27                   | 15              | 10              | 13              | 0               | 65    | 0.77     | 4.77    | 0.81                | 0.45       |
| 18       | 25                   | 18              | 12              | 11              | 0               | 66    | 0.88     | 3.49    | 0.78                | 0.64       |
| 19       | 28                   | 17              | 11              | 17              | 0               | 73    | 0.84     | 5.01    | 0.85                | 0.58       |
| 20       | 30                   | 18              | 11              | 16              | 0               | 75    | 0.78     | 3.46    | 0.73                | 0.57       |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

### 9.3 Distance violation statistics for the ensemble

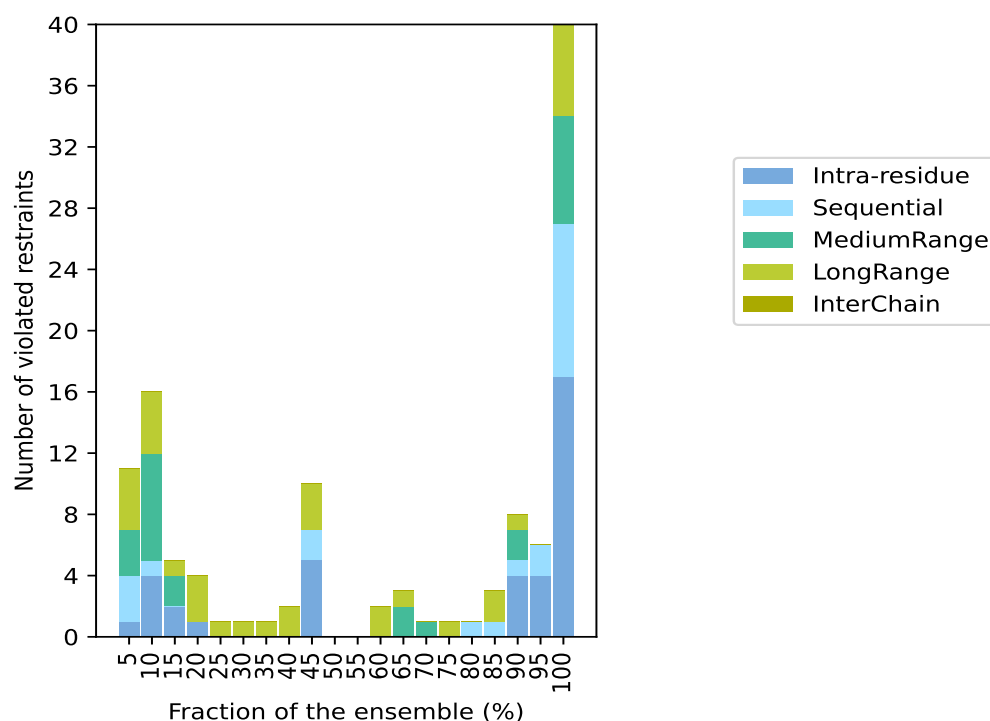
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 373(IR:218, SQ:95, MR:42, LR:18, IC:0) restraints are not 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>       | %     |
| 1                             | 3               | 3               | 4               | 0               | 11    | 1                        | 5.0   |
| 4                             | 1               | 7               | 4               | 0               | 16    | 2                        | 10.0  |
| 2                             | 0               | 2               | 1               | 0               | 5     | 3                        | 15.0  |
| 1                             | 0               | 0               | 3               | 0               | 4     | 4                        | 20.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 5                        | 25.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 6                        | 30.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 7                        | 35.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 8                        | 40.0  |
| 5                             | 2               | 0               | 3               | 0               | 10    | 9                        | 45.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 10                       | 50.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 55.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 12                       | 60.0  |
| 0                             | 0               | 2               | 1               | 0               | 3     | 13                       | 65.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 14                       | 70.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 15                       | 75.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 16                       | 80.0  |
| 0                             | 1               | 0               | 2               | 0               | 3     | 17                       | 85.0  |
| 4                             | 1               | 2               | 1               | 0               | 8     | 18                       | 90.0  |
| 4                             | 2               | 0               | 0               | 0               | 6     | 19                       | 95.0  |
| 17                            | 10              | 7               | 6               | 0               | 40    | 20                       | 100.0 |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

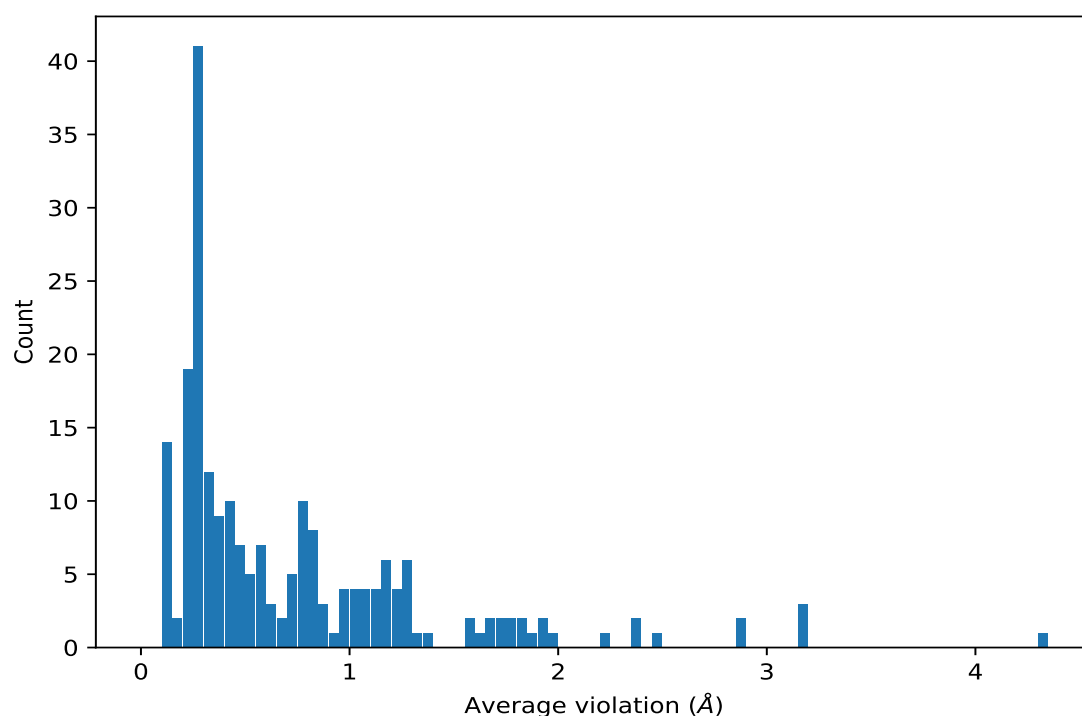
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 20                  | 4.3      | 0.63                | 4.43       |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD12 | 20                  | 3.15     | 0.95                | 2.85       |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD11 | 20                  | 3.15     | 0.95                | 2.85       |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD13 | 20                  | 3.15     | 0.95                | 2.85       |
| (2,31)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HD2   | 20                  | 2.88     | 0.34                | 2.88       |
| (2,31)  | 1:27:A:4PH:HD2 | 1:34:A:4PH:HB2  | 20                  | 2.88     | 0.34                | 2.88       |
| (1,356) | 1:28:A:GLN:HG2 | 1:27:A:4PH:HD1  | 20                  | 2.45     | 0.29                | 2.48       |
| (1,355) | 1:28:A:GLN:HG3 | 1:27:A:4PH:HD1  | 20                  | 2.23     | 0.8                 | 1.76       |
| (2,102) | 1:4:A:LYS:H    | 1:27:A:4PH:HD2  | 20                  | 1.96     | 0.37                | 2.0        |
| (2,103) | 1:4:A:LYS:H    | 1:27:A:4PH:HE2  | 20                  | 1.88     | 0.44                | 1.86       |
| (1,140) | 1:15:A:GLU:HG3 | 1:14:A:PRO:HD3  | 20                  | 1.64     | 0.53                | 1.6        |
| (1,349) | 1:18:A:ALA:HA  | 1:17:A:LEU:HB2  | 20                  | 1.26     | 0.02                | 1.27       |
| (2,62)  | 1:27:A:4PH:HD2 | 1:4:A:LYS:HG3   | 20                  | 1.26     | 0.37                | 1.37       |
| (2,62)  | 1:27:A:4PH:HD1 | 1:4:A:LYS:HG3   | 20                  | 1.26     | 0.37                | 1.37       |
| (2,91)  | 1:20:A:4PH:HB2 | 1:19:A:LYS:HG2  | 20                  | 1.21     | 0.19                | 1.22       |
| (2,91)  | 1:20:A:4PH:HB2 | 1:19:A:LYS:HG3  | 20                  | 1.21     | 0.19                | 1.22       |

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| Key     | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,9)   | 1:6:A:THR:HA   | 1:6:A:THR:HG21  | 20                  | 1.12     | 0.02                | 1.12       |
| (1,9)   | 1:6:A:THR:HA   | 1:6:A:THR:HG22  | 20                  | 1.12     | 0.02                | 1.12       |
| (1,9)   | 1:6:A:THR:HA   | 1:6:A:THR:HG23  | 20                  | 1.12     | 0.02                | 1.12       |
| (1,46)  | 1:5:A:PRO:HG2  | 1:4:A:LYS:HG3   | 20                  | 1.09     | 0.51                | 1.02       |
| (2,111) | 1:4:A:LYS:HA   | 1:24:A:LEU:H    | 20                  | 1.08     | 0.2                 | 1.1        |
| (2,111) | 1:8:A:PRO:HD3  | 1:24:A:LEU:H    | 20                  | 1.08     | 0.2                 | 1.1        |
| (2,111) | 1:11:A:ASN:HB2 | 1:15:A:GLU:H    | 20                  | 1.08     | 0.2                 | 1.1        |
| (1,48)  | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD12 | 20                  | 1.02     | 0.01                | 1.02       |
| (1,48)  | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD11 | 20                  | 1.02     | 0.01                | 1.02       |
| (1,48)  | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD13 | 20                  | 1.02     | 0.01                | 1.02       |
| (1,122) | 1:3:A:THR:HG21 | 1:4:A:LYS:H     | 20                  | 0.97     | 0.18                | 0.98       |
| (1,122) | 1:3:A:THR:HG23 | 1:4:A:LYS:H     | 20                  | 0.97     | 0.18                | 0.98       |
| (1,122) | 1:3:A:THR:HG22 | 1:4:A:LYS:H     | 20                  | 0.97     | 0.18                | 0.98       |
| (1,196) | 1:27:A:4PH:HD2 | 1:27:A:4PH:HA   | 20                  | 0.92     | 0.02                | 0.92       |
| (1,188) | 1:28:A:GLN:H   | 1:27:A:4PH:HD1  | 20                  | 0.82     | 0.05                | 0.81       |
| (2,55)  | 1:27:A:4PH:HD1 | 1:27:A:4PH:H33A | 20                  | 0.75     | 0.01                | 0.75       |
| (2,55)  | 1:27:A:4PH:HD2 | 1:27:A:4PH:H33B | 20                  | 0.75     | 0.01                | 0.75       |
| (2,55)  | 1:27:A:4PH:HD2 | 1:27:A:4PH:H33A | 20                  | 0.75     | 0.01                | 0.75       |
| (2,55)  | 1:27:A:4PH:HD1 | 1:27:A:4PH:H33B | 20                  | 0.75     | 0.01                | 0.75       |
| (2,55)  | 1:27:A:4PH:HD2 | 1:27:A:4PH:H33  | 20                  | 0.75     | 0.01                | 0.75       |
| (1,267) | 1:26:A:LYS:HB3 | 1:23:A:ASP:HA   | 20                  | 0.68     | 0.24                | 0.66       |
| (1,313) | 1:25:A:ALA:HA  | 1:28:A:GLN:HB3  | 20                  | 0.6      | 0.15                | 0.6        |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2  | 20                  | 0.59     | 0.01                | 0.6        |
| (1,322) | 1:19:A:LYS:HG2 | 1:19:A:LYS:H    | 20                  | 0.59     | 0.08                | 0.57       |
| (1,297) | 1:21:A:GLN:HA  | 1:24:A:LEU:HB3  | 20                  | 0.52     | 0.15                | 0.49       |
| (2,42)  | 1:21:A:GLN:H   | 1:22:A:ALA:HB1  | 20                  | 0.52     | 0.04                | 0.5        |
| (2,42)  | 1:21:A:GLN:H   | 1:22:A:ALA:HB3  | 20                  | 0.52     | 0.04                | 0.5        |
| (2,42)  | 1:21:A:GLN:H   | 1:22:A:ALA:HB2  | 20                  | 0.52     | 0.04                | 0.5        |
| (1,242) | 1:14:A:PRO:HD3 | 1:13:A:THR:HB   | 20                  | 0.48     | 0.1                 | 0.48       |
| (1,80)  | 1:27:A:4PH:HD1 | 1:24:A:LEU:HA   | 20                  | 0.47     | 0.12                | 0.46       |
| (1,49)  | 1:8:A:PRO:HB3  | 1:12:A:ALA:HB2  | 20                  | 0.43     | 0.13                | 0.42       |
| (1,49)  | 1:8:A:PRO:HB3  | 1:12:A:ALA:HB1  | 20                  | 0.43     | 0.13                | 0.42       |
| (1,49)  | 1:8:A:PRO:HB3  | 1:12:A:ALA:HB3  | 20                  | 0.43     | 0.13                | 0.42       |
| (1,345) | 1:8:A:PRO:HB3  | 1:8:A:PRO:HD2   | 20                  | 0.39     | 0.01                | 0.39       |
| (1,219) | 1:15:A:GLU:H   | 1:15:A:GLU:HB3  | 20                  | 0.35     | 0.02                | 0.35       |
| (1,240) | 1:20:A:4PH:HD1 | 1:21:A:GLN:HE21 | 20                  | 0.34     | 0.11                | 0.35       |
| (1,240) | 1:20:A:4PH:HD2 | 1:21:A:GLN:HE21 | 20                  | 0.34     | 0.11                | 0.35       |
| (1,264) | 1:26:A:LYS:H   | 1:26:A:LYS:HB3  | 20                  | 0.32     | 0.01                | 0.32       |
| (2,71)  | 1:34:A:4PH:H   | 1:34:A:4PH:HD1  | 20                  | 0.3      | 0.04                | 0.32       |
| (2,71)  | 1:34:A:4PH:H   | 1:34:A:4PH:HD2  | 20                  | 0.3      | 0.04                | 0.32       |
| (2,71)  | 1:20:A:4PH:H   | 1:20:A:4PH:HD2  | 20                  | 0.3      | 0.04                | 0.32       |
| (2,71)  | 1:20:A:4PH:H   | 1:20:A:4PH:HD1  | 20                  | 0.3      | 0.04                | 0.32       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,38)  | 1:27:A:4PH:HE1  | 1:27:A:4PH:H33A | 20                  | 0.29     | 0.0                 | 0.29       |
| (2,38)  | 1:27:A:4PH:HE2  | 1:27:A:4PH:H33B | 20                  | 0.29     | 0.0                 | 0.29       |
| (2,38)  | 1:27:A:4PH:HE2  | 1:27:A:4PH:H33A | 20                  | 0.29     | 0.0                 | 0.29       |
| (2,38)  | 1:27:A:4PH:HE2  | 1:27:A:4PH:H33  | 20                  | 0.29     | 0.0                 | 0.29       |
| (2,38)  | 1:27:A:4PH:HE1  | 1:27:A:4PH:H33B | 20                  | 0.29     | 0.0                 | 0.29       |
| (2,38)  | 1:27:A:4PH:HE1  | 1:27:A:4PH:H33  | 20                  | 0.29     | 0.0                 | 0.29       |
| (1,43)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HD12 | 20                  | 0.25     | 0.02                | 0.25       |
| (1,43)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HD12 | 20                  | 0.25     | 0.02                | 0.25       |
| (1,43)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HD11 | 20                  | 0.25     | 0.02                | 0.25       |
| (1,43)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HD13 | 20                  | 0.25     | 0.02                | 0.25       |
| (1,43)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HD11 | 20                  | 0.25     | 0.02                | 0.25       |
| (1,43)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HD13 | 20                  | 0.25     | 0.02                | 0.25       |
| (1,43)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HD12 | 20                  | 0.25     | 0.02                | 0.25       |
| (1,43)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HD13 | 20                  | 0.25     | 0.02                | 0.25       |
| (1,43)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HD11 | 20                  | 0.25     | 0.02                | 0.25       |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33B | 20                  | 0.24     | 0.01                | 0.24       |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33  | 20                  | 0.24     | 0.01                | 0.24       |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33A | 20                  | 0.24     | 0.01                | 0.24       |
| (2,39)  | 1:20:A:4PH:HE2  | 1:20:A:4PH:H33B | 20                  | 0.24     | 0.01                | 0.24       |
| (2,39)  | 1:20:A:4PH:HE2  | 1:20:A:4PH:H33  | 20                  | 0.24     | 0.01                | 0.24       |
| (2,39)  | 1:20:A:4PH:HE2  | 1:20:A:4PH:H33A | 20                  | 0.24     | 0.01                | 0.24       |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 20                  | 0.2      | 0.02                | 0.2        |
| (1,25)  | 1:18:A:ALA:HA   | 1:18:A:ALA:HB3  | 20                  | 0.14     | 0.01                | 0.14       |
| (1,25)  | 1:18:A:ALA:HA   | 1:18:A:ALA:HB2  | 20                  | 0.14     | 0.01                | 0.14       |
| (1,25)  | 1:18:A:ALA:HA   | 1:18:A:ALA:HB1  | 20                  | 0.14     | 0.01                | 0.14       |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 20                  | 0.14     | 0.01                | 0.14       |
| (1,24)  | 1:22:A:ALA:HB3  | 1:22:A:ALA:HA   | 20                  | 0.13     | 0.01                | 0.13       |
| (1,24)  | 1:22:A:ALA:HB2  | 1:22:A:ALA:HA   | 20                  | 0.13     | 0.01                | 0.13       |
| (1,24)  | 1:22:A:ALA:HB1  | 1:22:A:ALA:HA   | 20                  | 0.13     | 0.01                | 0.13       |
| (1,52)  | 1:0:A:ACE:H2    | 1:1:A:PRO:HD2   | 19                  | 0.47     | 0.16                | 0.5        |
| (1,52)  | 1:0:A:ACE:H1    | 1:1:A:PRO:HD2   | 19                  | 0.47     | 0.16                | 0.5        |
| (1,52)  | 1:0:A:ACE:H3    | 1:1:A:PRO:HD2   | 19                  | 0.47     | 0.16                | 0.5        |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 19                  | 0.45     | 0.01                | 0.45       |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 19                  | 0.3      | 0.1                 | 0.25       |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB1  | 19                  | 0.28     | 0.03                | 0.29       |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB3  | 19                  | 0.28     | 0.03                | 0.29       |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB2  | 19                  | 0.28     | 0.03                | 0.29       |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 19                  | 0.21     | 0.01                | 0.21       |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 19                  | 0.15     | 0.03                | 0.16       |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD23 | 18                  | 1.29     | 0.68                | 1.0        |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD21 | 18                  | 1.29     | 0.68                | 1.0        |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD22 | 18                  | 1.29     | 0.68                | 1.0        |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,42)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HB3  | 18                  | 1.17     | 0.01                | 1.17       |
| (1,42)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HB3  | 18                  | 1.17     | 0.01                | 1.17       |
| (1,42)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HB3  | 18                  | 1.17     | 0.01                | 1.17       |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD22 | 18                  | 0.87     | 0.25                | 0.89       |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD23 | 18                  | 0.87     | 0.25                | 0.89       |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD21 | 18                  | 0.87     | 0.25                | 0.89       |
| (1,44)  | 1:31:A:LEU:HD11 | 1:31:A:LEU:HB2  | 18                  | 0.71     | 0.01                | 0.71       |
| (1,44)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HB2  | 18                  | 0.71     | 0.01                | 0.71       |
| (1,44)  | 1:31:A:LEU:HD12 | 1:31:A:LEU:HB2  | 18                  | 0.71     | 0.01                | 0.71       |
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 18                  | 0.46     | 0.33                | 0.3        |
| (1,257) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3  | 18                  | 0.34     | 0.02                | 0.34       |
| (1,257) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3  | 18                  | 0.34     | 0.02                | 0.34       |
| (1,257) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3  | 18                  | 0.34     | 0.02                | 0.34       |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD13 | 18                  | 0.29     | 0.01                | 0.29       |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD12 | 18                  | 0.29     | 0.01                | 0.29       |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD11 | 18                  | 0.29     | 0.01                | 0.29       |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 18                  | 0.26     | 0.07                | 0.26       |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33A | 17                  | 0.83     | 0.27                | 0.9        |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33B | 17                  | 0.83     | 0.27                | 0.9        |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33  | 17                  | 0.83     | 0.27                | 0.9        |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H1    | 17                  | 0.76     | 0.36                | 0.75       |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H3    | 17                  | 0.76     | 0.36                | 0.75       |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H2    | 17                  | 0.76     | 0.36                | 0.75       |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG21  | 17                  | 0.37     | 0.18                | 0.35       |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG22  | 17                  | 0.37     | 0.18                | 0.35       |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG23  | 17                  | 0.37     | 0.18                | 0.35       |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 16                  | 0.39     | 0.31                | 0.31       |
| (1,372) | 1:27:A:4PH:HE1  | 1:4:A:LYS:HG2   | 15                  | 0.64     | 0.21                | 0.66       |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD22 | 14                  | 0.56     | 0.42                | 0.4        |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD23 | 14                  | 0.56     | 0.42                | 0.4        |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD21 | 14                  | 0.56     | 0.42                | 0.4        |
| (1,91)  | 1:27:A:4PH:HE1  | 1:2:A:PRO:HB3   | 13                  | 0.36     | 0.14                | 0.29       |
| (1,112) | 1:20:A:4PH:HD1  | 1:17:A:LEU:HD23 | 13                  | 0.28     | 0.13                | 0.23       |
| (1,112) | 1:20:A:4PH:HD2  | 1:17:A:LEU:HD22 | 13                  | 0.28     | 0.13                | 0.23       |
| (1,112) | 1:20:A:4PH:HD2  | 1:17:A:LEU:HD21 | 13                  | 0.28     | 0.13                | 0.23       |
| (1,112) | 1:20:A:4PH:HD1  | 1:17:A:LEU:HD21 | 13                  | 0.28     | 0.13                | 0.23       |
| (1,112) | 1:20:A:4PH:HD2  | 1:17:A:LEU:HD23 | 13                  | 0.28     | 0.13                | 0.23       |
| (1,112) | 1:20:A:4PH:HD1  | 1:17:A:LEU:HD22 | 13                  | 0.28     | 0.13                | 0.23       |
| (1,296) | 1:31:A:LEU:HD22 | 1:27:A:4PH:H33  | 13                  | 0.26     | 0.13                | 0.24       |
| (1,296) | 1:31:A:LEU:HD23 | 1:27:A:4PH:H33  | 13                  | 0.26     | 0.13                | 0.24       |
| (1,296) | 1:31:A:LEU:HD21 | 1:27:A:4PH:H33  | 13                  | 0.26     | 0.13                | 0.24       |
| (1,296) | 1:31:A:LEU:HD21 | 1:27:A:4PH:H33B | 13                  | 0.26     | 0.13                | 0.24       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,296) | 1:31:A:LEU:HD23 | 1:27:A:4PH:H33A | 13                  | 0.26     | 0.13                | 0.24       |
| (1,296) | 1:31:A:LEU:HD22 | 1:27:A:4PH:H33A | 13                  | 0.26     | 0.13                | 0.24       |
| (1,296) | 1:31:A:LEU:HD21 | 1:27:A:4PH:H33A | 13                  | 0.26     | 0.13                | 0.24       |
| (1,296) | 1:31:A:LEU:HD22 | 1:27:A:4PH:H33B | 13                  | 0.26     | 0.13                | 0.24       |
| (1,32)  | 1:34:A:4PH:HB3  | 1:2:A:PRO:HG2   | 12                  | 0.62     | 0.21                | 0.53       |
| (2,41)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HB3   | 12                  | 0.53     | 0.29                | 0.5        |
| (1,125) | 1:21:A:GLN:HG2  | 1:20:A:4PH:HD2  | 9                   | 1.36     | 0.12                | 1.28       |
| (1,206) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG3   | 9                   | 1.32     | 0.22                | 1.3        |
| (1,151) | 1:21:A:GLN:HE22 | 1:20:A:4PH:HD2  | 9                   | 1.12     | 0.21                | 1.08       |
| (1,194) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HA   | 9                   | 1.02     | 0.03                | 1.02       |
| (1,77)  | 1:34:A:4PH:HD1  | 1:34:A:4PH:HA   | 9                   | 0.97     | 0.05                | 0.96       |
| (1,83)  | 1:20:A:4PH:HD2  | 1:20:A:4PH:HB2  | 9                   | 0.82     | 0.01                | 0.82       |
| (1,152) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG2   | 9                   | 0.66     | 0.18                | 0.65       |
| (2,66)  | 1:20:A:4PH:HD1  | 1:5:A:PRO:HG2   | 9                   | 0.59     | 0.17                | 0.62       |
| (2,66)  | 1:20:A:4PH:HD1  | 1:24:A:LEU:HB3  | 9                   | 0.59     | 0.17                | 0.62       |
| (1,239) | 1:34:A:4PH:HB2  | 1:34:A:4PH:HD2  | 9                   | 0.4      | 0.01                | 0.4        |
| (1,195) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HB3  | 9                   | 0.27     | 0.02                | 0.27       |
| (2,13)  | 1:24:A:LEU:HD11 | 1:5:A:PRO:HG2   | 8                   | 0.41     | 0.19                | 0.41       |
| (2,13)  | 1:24:A:LEU:HD13 | 1:5:A:PRO:HG2   | 8                   | 0.41     | 0.19                | 0.41       |
| (2,13)  | 1:24:A:LEU:HD12 | 1:5:A:PRO:HG2   | 8                   | 0.41     | 0.19                | 0.41       |
| (1,93)  | 1:34:A:4PH:HD1  | 1:0:A:ACE:H2    | 8                   | 0.23     | 0.11                | 0.2        |
| (1,93)  | 1:34:A:4PH:HD2  | 1:0:A:ACE:H3    | 8                   | 0.23     | 0.11                | 0.2        |
| (1,93)  | 1:34:A:4PH:HD1  | 1:0:A:ACE:H1    | 8                   | 0.23     | 0.11                | 0.2        |
| (1,93)  | 1:34:A:4PH:HD2  | 1:0:A:ACE:H1    | 8                   | 0.23     | 0.11                | 0.2        |
| (1,93)  | 1:34:A:4PH:HD2  | 1:0:A:ACE:H2    | 8                   | 0.23     | 0.11                | 0.2        |
| (1,93)  | 1:34:A:4PH:HD1  | 1:0:A:ACE:H3    | 8                   | 0.23     | 0.11                | 0.2        |
| (2,36)  | 1:8:A:PRO:HD3   | 1:20:A:4PH:HD2  | 7                   | 0.22     | 0.16                | 0.13       |
| (2,36)  | 1:8:A:PRO:HD3   | 1:20:A:4PH:HD1  | 7                   | 0.22     | 0.16                | 0.13       |
| (1,34)  | 1:5:A:PRO:HD2   | 1:24:A:LEU:HD11 | 6                   | 0.83     | 0.91                | 0.26       |
| (1,34)  | 1:5:A:PRO:HD2   | 1:24:A:LEU:HD13 | 6                   | 0.83     | 0.91                | 0.26       |
| (1,34)  | 1:5:A:PRO:HD2   | 1:24:A:LEU:HD12 | 6                   | 0.83     | 0.91                | 0.26       |
| (1,74)  | 1:3:A:THR:HA    | 1:27:A:4PH:HE1  | 5                   | 0.27     | 0.12                | 0.27       |
| (2,85)  | 1:8:A:PRO:HD2   | 1:20:A:4PH:HD2  | 4                   | 0.44     | 0.33                | 0.31       |
| (2,85)  | 1:8:A:PRO:HD2   | 1:20:A:4PH:HD1  | 4                   | 0.44     | 0.33                | 0.31       |
| (1,373) | 1:27:A:4PH:HD2  | 1:4:A:LYS:HA    | 4                   | 0.31     | 0.16                | 0.3        |
| (1,364) | 1:0:A:ACE:H3    | 1:34:A:4PH:HB3  | 4                   | 0.25     | 0.08                | 0.24       |
| (1,364) | 1:0:A:ACE:H2    | 1:34:A:4PH:HB3  | 4                   | 0.25     | 0.08                | 0.24       |
| (1,12)  | 1:17:A:LEU:HA   | 1:17:A:LEU:HD23 | 4                   | 0.12     | 0.02                | 0.12       |
| (1,12)  | 1:17:A:LEU:HA   | 1:17:A:LEU:HD22 | 4                   | 0.12     | 0.02                | 0.12       |
| (2,49)  | 1:20:A:4PH:HD2  | 1:24:A:LEU:HD21 | 3                   | 1.17     | 0.75                | 1.67       |
| (2,49)  | 1:20:A:4PH:HD2  | 1:24:A:LEU:HD12 | 3                   | 1.17     | 0.75                | 1.67       |
| (2,49)  | 1:20:A:4PH:HD2  | 1:24:A:LEU:HD23 | 3                   | 1.17     | 0.75                | 1.67       |

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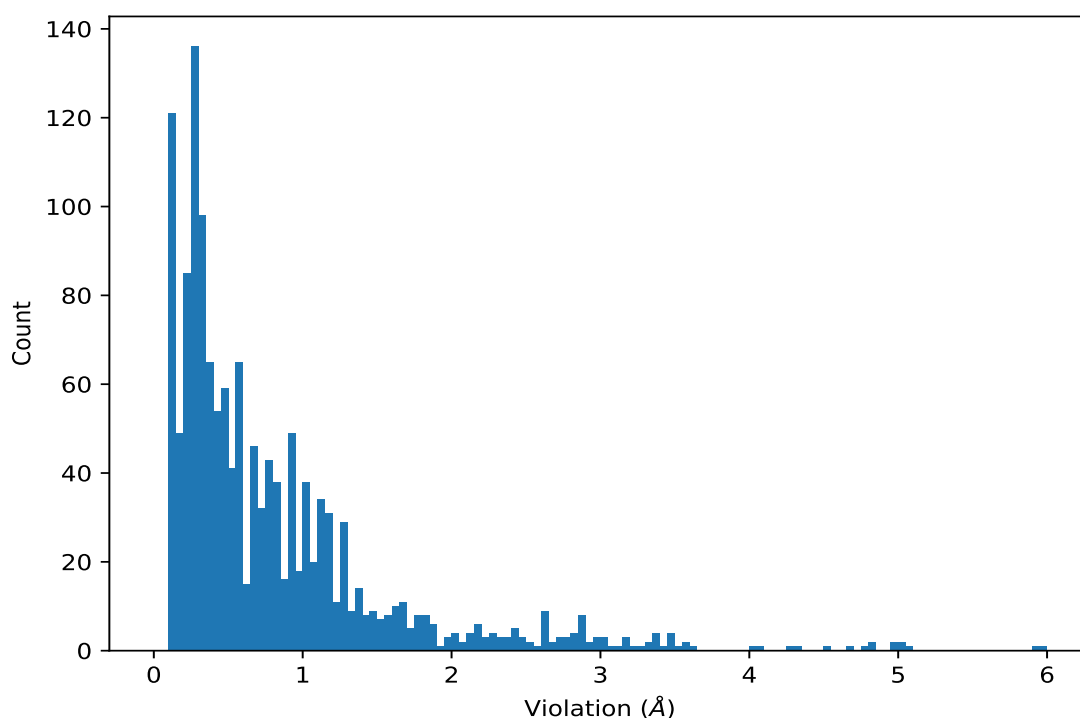
| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,110) | 1:27:A:4PH:HD2  | 1:5:A:PRO:HG2   | 3                   | 0.44     | 0.38                | 0.17       |
| (2,74)  | 1:20:A:4PH:HD1  | 1:20:A:4PH:HB3  | 3                   | 0.29     | 0.02                | 0.3        |
| (1,209) | 1:20:A:4PH:HE1  | 1:7:A:LYS:HA    | 3                   | 0.22     | 0.14                | 0.13       |
| (1,266) | 1:26:A:LYS:HG2  | 1:26:A:LYS:H    | 3                   | 0.21     | 0.02                | 0.19       |
| (1,118) | 1:24:A:LEU:HD13 | 1:27:A:4PH:HD2  | 2                   | 2.38     | 0.03                | 2.38       |
| (1,118) | 1:24:A:LEU:HD12 | 1:27:A:4PH:HD2  | 2                   | 2.38     | 0.03                | 2.38       |
| (2,11)  | 1:34:A:4PH:HB2  | 1:31:A:LEU:HD21 | 2                   | 1.9      | 0.27                | 1.9        |
| (2,11)  | 1:34:A:4PH:HB2  | 1:31:A:LEU:HD23 | 2                   | 1.9      | 0.27                | 1.9        |
| (1,17)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HA   | 2                   | 1.84     | 0.03                | 1.84       |
| (1,17)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HA   | 2                   | 1.84     | 0.03                | 1.84       |
| (1,33)  | 1:27:A:4PH:HB2  | 1:24:A:LEU:HD13 | 2                   | 1.78     | 0.01                | 1.78       |
| (1,33)  | 1:27:A:4PH:HB2  | 1:24:A:LEU:HD12 | 2                   | 1.78     | 0.01                | 1.78       |
| (1,15)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD13 | 2                   | 1.72     | 0.02                | 1.72       |
| (1,15)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD12 | 2                   | 1.72     | 0.02                | 1.72       |
| (1,16)  | 1:24:A:LEU:HD23 | 1:21:A:GLN:HA   | 2                   | 1.66     | 0.12                | 1.66       |
| (1,16)  | 1:24:A:LEU:HD21 | 1:21:A:GLN:HA   | 2                   | 1.66     | 0.12                | 1.66       |
| (1,119) | 1:34:A:4PH:HD2  | 1:31:A:LEU:HD21 | 2                   | 1.56     | 0.48                | 1.56       |
| (1,119) | 1:34:A:4PH:HD2  | 1:31:A:LEU:HD23 | 2                   | 1.56     | 0.48                | 1.56       |
| (1,141) | 1:5:A:PRO:HD3   | 1:24:A:LEU:HD12 | 2                   | 1.22     | 0.09                | 1.22       |
| (1,141) | 1:5:A:PRO:HD3   | 1:24:A:LEU:HD11 | 2                   | 1.22     | 0.09                | 1.22       |
| (2,56)  | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD21 | 2                   | 0.75     | 0.08                | 0.75       |
| (2,56)  | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD23 | 2                   | 0.75     | 0.08                | 0.75       |
| (2,10)  | 1:7:A:LYS:HA    | 1:24:A:LEU:HD12 | 2                   | 0.7      | 0.05                | 0.7        |
| (2,10)  | 1:7:A:LYS:HA    | 1:24:A:LEU:HD11 | 2                   | 0.7      | 0.05                | 0.7        |
| (2,50)  | 1:27:A:4PH:HD2  | 1:31:A:LEU:HD23 | 2                   | 0.38     | 0.15                | 0.38       |
| (2,50)  | 1:27:A:4PH:HD2  | 1:31:A:LEU:HD22 | 2                   | 0.38     | 0.15                | 0.38       |
| (2,20)  | 1:18:A:ALA:HB3  | 1:15:A:GLU:HA   | 2                   | 0.24     | 0.01                | 0.24       |
| (2,27)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HA    | 2                   | 0.18     | 0.08                | 0.18       |
| (2,48)  | 1:25:A:ALA:H    | 1:24:A:LEU:HD22 | 2                   | 0.12     | 0.01                | 0.12       |
| (2,48)  | 1:25:A:ALA:H    | 1:24:A:LEU:HD21 | 2                   | 0.12     | 0.01                | 0.12       |
| (2,67)  | 1:7:A:LYS:H     | 1:7:A:LYS:HD2   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,104) | 1:13:A:THR:H    | 1:13:A:THR:HG22 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,104) | 1:13:A:THR:H    | 1:13:A:THR:HG21 | 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 [i](#)

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

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



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

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

| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD13 | 16       | 5.98          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD12 | 11       | 5.91          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 6        | 5.08          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 9        | 5.01          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 19       | 5.01          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 3        | 4.97          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 2        | 4.96          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 13       | 4.84          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 11       | 4.82          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 17       | 4.77          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 14       | 4.67          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 16       | 4.51          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 4        | 4.35          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 15       | 4.29          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 12       | 4.07          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 10       | 4.0           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 7        | 3.63          |
| (1,355) | 1:28:A:GLN:HG3 | 1:27:A:4PH:HD1  | 11       | 3.59          |
| (1,140) | 1:15:A:GLU:HG3 | 1:14:A:PRO:HD3  | 1        | 3.59          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 8        | 3.54          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 18       | 3.49          |
| (1,355) | 1:28:A:GLN:HG3 | 1:27:A:4PH:HD1  | 15       | 3.48          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 5        | 3.47          |
| (1,355) | 1:28:A:GLN:HG3 | 1:27:A:4PH:HD1  | 20       | 3.46          |
| (1,355) | 1:28:A:GLN:HG3 | 1:27:A:4PH:HD1  | 12       | 3.43          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 20       | 3.38          |
| (2,31)  | 1:27:A:4PH:HD2 | 1:34:A:4PH:HB2  | 19       | 3.37          |
| (2,31)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HD2   | 3        | 3.36          |
| (1,355) | 1:28:A:GLN:HG3 | 1:27:A:4PH:HD1  | 18       | 3.35          |
| (2,31)  | 1:27:A:4PH:HD2 | 1:34:A:4PH:HB2  | 11       | 3.33          |
| (1,355) | 1:28:A:GLN:HG3 | 1:27:A:4PH:HD1  | 19       | 3.31          |
| (2,31)  | 1:27:A:4PH:HD2 | 1:34:A:4PH:HB2  | 14       | 3.27          |
| (1,90)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HB3   | 1        | 3.21          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD13 | 4        | 3.19          |
| (2,31)  | 1:27:A:4PH:HD2 | 1:34:A:4PH:HB2  | 2        | 3.18          |
| (2,31)  | 1:27:A:4PH:HD2 | 1:34:A:4PH:HB2  | 4        | 3.18          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD11 | 7        | 3.12          |
| (2,31)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HD2   | 9        | 3.06          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD11 | 5        | 3.05          |
| (2,31)  | 1:27:A:4PH:HD2 | 1:34:A:4PH:HB2  | 15       | 3.01          |
| (2,31)  | 1:27:A:4PH:HD2 | 1:34:A:4PH:HB2  | 17       | 3.0           |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD11 | 2        | 2.99          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD12 | 14       | 2.99          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD13 | 3        | 2.96          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD13 | 8        | 2.94          |
| (2,31)  | 1:27:A:4PH:HD2 | 1:34:A:4PH:HB2  | 13       | 2.92          |
| (1,356) | 1:28:A:GLN:HG2 | 1:27:A:4PH:HD1  | 10       | 2.88          |
| (1,46)  | 1:5:A:PRO:HG2  | 1:4:A:LYS:HG3   | 18       | 2.88          |
| (1,356) | 1:28:A:GLN:HG2 | 1:27:A:4PH:HD1  | 16       | 2.87          |
| (1,356) | 1:28:A:GLN:HG2 | 1:27:A:4PH:HD1  | 7        | 2.86          |
| (2,31)  | 1:27:A:4PH:HD2 | 1:2:A:PRO:HD2   | 16       | 2.85          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD11 | 6        | 2.85          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD13 | 9        | 2.85          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD11 | 19       | 2.85          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD11 | 17       | 2.84          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD13 | 18       | 2.84          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD13 | 10       | 2.82          |
| (1,132) | 1:27:A:4PH:HE1 | 1:24:A:LEU:HD12 | 20       | 2.81          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,31)  | 1:27:A:4PH:HD2  | 1:2:A:PRO:HD2   | 5        | 2.79          |
| (1,132) | 1:27:A:4PH:HE1  | 1:24:A:LEU:HD13 | 13       | 2.78          |
| (2,31)  | 1:27:A:4PH:HD2  | 1:2:A:PRO:HD2   | 8        | 2.75          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 5        | 2.72          |
| (2,31)  | 1:27:A:4PH:HD2  | 1:2:A:PRO:HD2   | 6        | 2.7           |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 4        | 2.7           |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD21 | 3        | 2.68          |
| (2,31)  | 1:27:A:4PH:HD2  | 1:2:A:PRO:HD2   | 10       | 2.66          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 1        | 2.63          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 2        | 2.63          |
| (1,132) | 1:27:A:4PH:HE1  | 1:24:A:LEU:HD12 | 12       | 2.62          |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD21 | 17       | 2.62          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 8        | 2.61          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 14       | 2.61          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 10       | 2.6           |
| (2,31)  | 1:27:A:4PH:HD2  | 1:2:A:PRO:HD2   | 7        | 2.6           |
| (2,31)  | 1:27:A:4PH:HD2  | 1:2:A:PRO:HD2   | 12       | 2.6           |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 10       | 2.56          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 15       | 2.54          |
| (2,31)  | 1:27:A:4PH:HD2  | 1:2:A:PRO:HD2   | 20       | 2.51          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 13       | 2.49          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 6        | 2.47          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 2        | 2.45          |
| (2,31)  | 1:27:A:4PH:HD2  | 1:2:A:PRO:HD2   | 18       | 2.43          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 3        | 2.43          |
| (1,132) | 1:27:A:4PH:HE1  | 1:24:A:LEU:HD12 | 1        | 2.43          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 2        | 2.42          |
| (1,118) | 1:24:A:LEU:HD13 | 1:27:A:4PH:HD2  | 16       | 2.42          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 15       | 2.38          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 7        | 2.36          |
| (1,118) | 1:24:A:LEU:HD12 | 1:27:A:4PH:HD2  | 11       | 2.35          |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD22 | 7        | 2.33          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 12       | 2.32          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 19       | 2.32          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 17       | 2.28          |
| (1,132) | 1:27:A:4PH:HE1  | 1:24:A:LEU:HD11 | 15       | 2.27          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 7        | 2.25          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 9        | 2.25          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 11       | 2.23          |
| (1,34)  | 1:5:A:PRO:HD2   | 1:24:A:LEU:HD12 | 16       | 2.22          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 12       | 2.21          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 16       | 2.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 20       | 2.17          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 13       | 2.16          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 16       | 2.16          |
| (2,11)  | 1:34:A:4PH:HB2  | 1:31:A:LEU:HD23 | 12       | 2.16          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 5        | 2.15          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 15       | 2.14          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 19       | 2.12          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 20       | 2.11          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 5        | 2.1           |
| (2,31)  | 1:27:A:4PH:HD2  | 1:2:A:PRO:HD2   | 1        | 2.07          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 12       | 2.06          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 16       | 2.05          |
| (1,119) | 1:34:A:4PH:HD2  | 1:31:A:LEU:HD23 | 12       | 2.05          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 20       | 2.03          |
| (1,34)  | 1:5:A:PRO:HD2   | 1:24:A:LEU:HD11 | 11       | 2.01          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 18       | 1.99          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 3        | 1.98          |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD21 | 4        | 1.96          |
| (1,356) | 1:28:A:GLN:HG2  | 1:27:A:4PH:HD1  | 19       | 1.94          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 3        | 1.88          |
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 13       | 1.88          |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD22 | 5        | 1.88          |
| (1,17)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HA   | 18       | 1.86          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 4        | 1.85          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 18       | 1.85          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 13       | 1.84          |
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 16       | 1.83          |
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 10       | 1.82          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 12       | 1.82          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 4        | 1.81          |
| (1,17)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HA   | 12       | 1.81          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 18       | 1.8           |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 20       | 1.8           |
| (1,33)  | 1:27:A:4PH:HB2  | 1:24:A:LEU:HD13 | 16       | 1.79          |
| (2,62)  | 1:27:A:4PH:HD2  | 1:4:A:LYS:HG3   | 13       | 1.78          |
| (1,33)  | 1:27:A:4PH:HB2  | 1:24:A:LEU:HD12 | 11       | 1.78          |
| (1,16)  | 1:24:A:LEU:HD21 | 1:21:A:GLN:HA   | 11       | 1.78          |
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 6        | 1.77          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 13       | 1.76          |
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 8        | 1.76          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 19       | 1.75          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 8        | 1.74          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 14       | 1.74          |
| (2,49)  | 1:20:A:4PH:HD2  | 1:24:A:LEU:HD21 | 11       | 1.73          |
| (1,15)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD13 | 16       | 1.73          |
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 7        | 1.71          |
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 4        | 1.7           |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 14       | 1.7           |
| (1,15)  | 1:24:A:LEU:HA   | 1:24:A:LEU:HD12 | 11       | 1.7           |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 9        | 1.69          |
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 1        | 1.68          |
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 3        | 1.68          |
| (2,62)  | 1:27:A:4PH:HD2  | 1:4:A:LYS:HG3   | 5        | 1.67          |
| (2,62)  | 1:27:A:4PH:HD1  | 1:4:A:LYS:HG3   | 19       | 1.67          |
| (2,49)  | 1:20:A:4PH:HD2  | 1:24:A:LEU:HD12 | 16       | 1.67          |
| (1,206) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG3   | 1        | 1.67          |
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 2        | 1.66          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 14       | 1.64          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 6        | 1.64          |
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 17       | 1.64          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 8        | 1.63          |
| (2,11)  | 1:34:A:4PH:HB2  | 1:31:A:LEU:HD21 | 18       | 1.63          |
| (1,206) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG3   | 18       | 1.63          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 4        | 1.61          |
| (1,125) | 1:21:A:GLN:HG2  | 1:20:A:4PH:HD2  | 3        | 1.61          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 6        | 1.6           |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 11       | 1.6           |
| (2,62)  | 1:27:A:4PH:HD1  | 1:4:A:LYS:HG3   | 15       | 1.59          |
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 5        | 1.59          |
| (2,62)  | 1:27:A:4PH:HD2  | 1:4:A:LYS:HG3   | 8        | 1.58          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 8        | 1.58          |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD23 | 11       | 1.57          |
| (2,111) | 1:4:A:LYS:HA    | 1:24:A:LEU:H    | 10       | 1.56          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 5        | 1.56          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 17       | 1.55          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG2  | 13       | 1.54          |
| (1,16)  | 1:24:A:LEU:HD23 | 1:21:A:GLN:HA   | 16       | 1.54          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 14       | 1.53          |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD22 | 14       | 1.53          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 11       | 1.51          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 14       | 1.51          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 17       | 1.5           |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG2  | 6        | 1.49          |
| (1,125) | 1:21:A:GLN:HG2  | 1:20:A:4PH:HD2  | 20       | 1.49          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 6        | 1.48          |
| (2,62)  | 1:27:A:4PH:HD1  | 1:4:A:LYS:HG3   | 12       | 1.48          |
| (1,355) | 1:28:A:GLN:HG3  | 1:27:A:4PH:HD1  | 9        | 1.48          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 20       | 1.48          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 9        | 1.47          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG2  | 2        | 1.47          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 4        | 1.47          |
| (2,62)  | 1:27:A:4PH:HD1  | 1:4:A:LYS:HG3   | 4        | 1.45          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 15       | 1.45          |
| (1,206) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG3   | 2        | 1.42          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 10       | 1.42          |
| (1,125) | 1:21:A:GLN:HG2  | 1:20:A:4PH:HD2  | 11       | 1.42          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG2  | 18       | 1.41          |
| (1,151) | 1:21:A:GLN:HE22 | 1:20:A:4PH:HD2  | 1        | 1.41          |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD21 | 16       | 1.41          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 17       | 1.4           |
| (2,62)  | 1:27:A:4PH:HD1  | 1:4:A:LYS:HG3   | 7        | 1.4           |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG2  | 5        | 1.39          |
| (2,62)  | 1:27:A:4PH:HD1  | 1:4:A:LYS:HG3   | 2        | 1.39          |
| (1,125) | 1:21:A:GLN:HG2  | 1:20:A:4PH:HD2  | 19       | 1.39          |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 18       | 1.39          |
| (2,102) | 1:4:A:LYS:H     | 1:27:A:4PH:HD2  | 1        | 1.38          |
| (2,62)  | 1:27:A:4PH:HD1  | 1:4:A:LYS:HG3   | 10       | 1.38          |
| (1,151) | 1:21:A:GLN:HE22 | 1:20:A:4PH:HD2  | 11       | 1.38          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H3    | 13       | 1.38          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG2  | 16       | 1.37          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 7        | 1.37          |
| (2,62)  | 1:27:A:4PH:HD2  | 1:4:A:LYS:HG3   | 3        | 1.36          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 12       | 1.36          |
| (1,206) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG3   | 11       | 1.33          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 2        | 1.32          |
| (2,62)  | 1:27:A:4PH:HD1  | 1:4:A:LYS:HG3   | 16       | 1.31          |
| (1,141) | 1:5:A:PRO:HD3   | 1:24:A:LEU:HD11 | 11       | 1.31          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 15       | 1.31          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 7        | 1.3           |
| (1,206) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG3   | 16       | 1.3           |
| (1,151) | 1:21:A:GLN:HE22 | 1:20:A:4PH:HD2  | 20       | 1.3           |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 7        | 1.3           |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 11       | 1.29          |
| (2,111) | 1:8:A:PRO:HD3   | 1:24:A:LEU:H    | 19       | 1.28          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 9        | 1.28          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 17       | 1.28          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,125) | 1:21:A:GLN:HG2  | 1:20:A:4PH:HD2  | 1        | 1.28          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD22 | 11       | 1.28          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG3  | 14       | 1.27          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG2  | 20       | 1.27          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 4        | 1.27          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 6        | 1.27          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 8        | 1.27          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 10       | 1.27          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 11       | 1.27          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 12       | 1.27          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 16       | 1.27          |
| (1,125) | 1:21:A:GLN:HG2  | 1:20:A:4PH:HD2  | 2        | 1.27          |
| (1,125) | 1:21:A:GLN:HG2  | 1:20:A:4PH:HD2  | 16       | 1.27          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33B | 7        | 1.27          |
| (2,111) | 1:11:A:ASN:HB2  | 1:15:A:GLU:H    | 13       | 1.26          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 14       | 1.26          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 19       | 1.26          |
| (1,125) | 1:21:A:GLN:HG2  | 1:20:A:4PH:HD2  | 18       | 1.26          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG3  | 19       | 1.25          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 1        | 1.25          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 5        | 1.25          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 13       | 1.25          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 15       | 1.25          |
| (1,151) | 1:21:A:GLN:HE22 | 1:20:A:4PH:HD2  | 2        | 1.25          |
| (1,125) | 1:21:A:GLN:HG2  | 1:20:A:4PH:HD2  | 14       | 1.25          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 1        | 1.24          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG3  | 11       | 1.24          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 3        | 1.24          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 2        | 1.23          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 18       | 1.23          |
| (1,349) | 1:18:A:ALA:HA   | 1:17:A:LEU:HB2  | 20       | 1.23          |
| (1,206) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG3   | 14       | 1.23          |
| (1,206) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG3   | 20       | 1.23          |
| (1,122) | 1:3:A:THR:HG21  | 1:4:A:LYS:H     | 3        | 1.23          |
| (2,111) | 1:8:A:PRO:HD3   | 1:24:A:LEU:H    | 15       | 1.22          |
| (1,122) | 1:3:A:THR:HG21  | 1:4:A:LYS:H     | 20       | 1.21          |
| (2,111) | 1:8:A:PRO:HD3   | 1:24:A:LEU:H    | 2        | 1.2           |
| (2,111) | 1:8:A:PRO:HD3   | 1:24:A:LEU:H    | 9        | 1.2           |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG3  | 4        | 1.2           |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG2  | 8        | 1.2           |
| (2,111) | 1:8:A:PRO:HD3   | 1:24:A:LEU:H    | 7        | 1.19          |
| (1,122) | 1:3:A:THR:HG23  | 1:4:A:LYS:H     | 5        | 1.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 5        | 1.19          |
| (2,111) | 1:8:A:PRO:HD3   | 1:24:A:LEU:H    | 14       | 1.18          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG2  | 3        | 1.18          |
| (1,42)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HB3  | 5        | 1.18          |
| (1,42)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HB3  | 8        | 1.18          |
| (1,42)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HB3  | 9        | 1.18          |
| (1,42)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HB3  | 10       | 1.18          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H2    | 9        | 1.18          |
| (1,42)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HB3  | 2        | 1.17          |
| (1,42)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HB3  | 3        | 1.17          |
| (1,42)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HB3  | 4        | 1.17          |
| (1,42)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HB3  | 6        | 1.17          |
| (1,42)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HB3  | 11       | 1.17          |
| (1,42)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HB3  | 15       | 1.17          |
| (1,42)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HB3  | 16       | 1.17          |
| (1,42)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HB3  | 17       | 1.17          |
| (1,42)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HB3  | 19       | 1.17          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33B | 10       | 1.17          |
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 8        | 1.16          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 6        | 1.16          |
| (1,42)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HB3  | 1        | 1.16          |
| (1,42)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HB3  | 7        | 1.16          |
| (1,42)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HB3  | 13       | 1.16          |
| (1,42)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HB3  | 14       | 1.16          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD22 | 5        | 1.16          |
| (2,111) | 1:4:A:LYS:HA    | 1:24:A:LEU:H    | 20       | 1.15          |
| (1,42)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HB3  | 20       | 1.15          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG23  | 10       | 1.15          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG21  | 11       | 1.15          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG22  | 14       | 1.15          |
| (1,122) | 1:3:A:THR:HG23  | 1:4:A:LYS:H     | 10       | 1.14          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG21  | 4        | 1.14          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG23  | 9        | 1.14          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG23  | 13       | 1.14          |
| (2,62)  | 1:27:A:4PH:HD2  | 1:4:A:LYS:HG3   | 14       | 1.13          |
| (1,122) | 1:3:A:THR:HG23  | 1:4:A:LYS:H     | 7        | 1.13          |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD21 | 18       | 1.13          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H3    | 19       | 1.13          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG21  | 2        | 1.13          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG22  | 3        | 1.13          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG21  | 5        | 1.13          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG21  | 19       | 1.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,141) | 1:5:A:PRO:HD3   | 1:24:A:LEU:HD12 | 16       | 1.12          |
| (1,122) | 1:3:A:THR:HG22  | 1:4:A:LYS:H     | 17       | 1.12          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG21  | 6        | 1.12          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG22  | 18       | 1.12          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG2  | 12       | 1.11          |
| (1,122) | 1:3:A:THR:HG21  | 1:4:A:LYS:H     | 1        | 1.11          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H2    | 3        | 1.11          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG21  | 7        | 1.11          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG21  | 12       | 1.11          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG23  | 15       | 1.11          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG22  | 16       | 1.11          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG21  | 17       | 1.11          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG21  | 20       | 1.11          |
| (2,111) | 1:8:A:PRO:HD3   | 1:24:A:LEU:H    | 3        | 1.1           |
| (2,111) | 1:8:A:PRO:HD3   | 1:24:A:LEU:H    | 5        | 1.1           |
| (1,122) | 1:3:A:THR:HG21  | 1:4:A:LYS:H     | 18       | 1.1           |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H1    | 11       | 1.1           |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG3  | 15       | 1.09          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD21 | 7        | 1.09          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD21 | 8        | 1.09          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG21  | 1        | 1.09          |
| (1,9)   | 1:6:A:THR:HA    | 1:6:A:THR:HG21  | 8        | 1.09          |
| (2,111) | 1:8:A:PRO:HD3   | 1:24:A:LEU:H    | 12       | 1.08          |
| (1,372) | 1:27:A:4PH:HE1  | 1:4:A:LYS:HG2   | 9        | 1.08          |
| (1,151) | 1:21:A:GLN:HE22 | 1:20:A:4PH:HD2  | 14       | 1.08          |
| (1,119) | 1:34:A:4PH:HD2  | 1:31:A:LEU:HD21 | 18       | 1.08          |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD22 | 19       | 1.08          |
| (2,62)  | 1:27:A:4PH:HD2  | 1:4:A:LYS:HG3   | 9        | 1.07          |
| (1,194) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HA   | 18       | 1.07          |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD23 | 1        | 1.07          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 13       | 1.07          |
| (2,62)  | 1:27:A:4PH:HD2  | 1:4:A:LYS:HG3   | 6        | 1.06          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H2    | 17       | 1.06          |
| (2,62)  | 1:27:A:4PH:HD2  | 1:4:A:LYS:HG3   | 17       | 1.05          |
| (2,41)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HB3   | 9        | 1.05          |
| (1,194) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HA   | 14       | 1.05          |
| (1,194) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HA   | 16       | 1.05          |
| (2,111) | 1:8:A:PRO:HD3   | 1:24:A:LEU:H    | 4        | 1.03          |
| (1,194) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HA   | 19       | 1.03          |
| (1,122) | 1:3:A:THR:HG23  | 1:4:A:LYS:H     | 11       | 1.03          |
| (1,77)  | 1:34:A:4PH:HD1  | 1:34:A:4PH:HA   | 2        | 1.03          |
| (1,77)  | 1:34:A:4PH:HD1  | 1:34:A:4PH:HA   | 11       | 1.03          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD12 | 4        | 1.03          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD11 | 6        | 1.03          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD11 | 7        | 1.03          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD12 | 10       | 1.03          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 16       | 1.03          |
| (1,32)  | 1:34:A:4PH:HB3  | 1:2:A:PRO:HG2   | 14       | 1.03          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD22 | 4        | 1.03          |
| (1,206) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG3   | 3        | 1.02          |
| (1,194) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HA   | 3        | 1.02          |
| (1,194) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HA   | 11       | 1.02          |
| (1,194) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HA   | 20       | 1.02          |
| (1,77)  | 1:34:A:4PH:HD1  | 1:34:A:4PH:HA   | 5        | 1.02          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD11 | 3        | 1.02          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD12 | 9        | 1.02          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD12 | 11       | 1.02          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD12 | 13       | 1.02          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD13 | 15       | 1.02          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD13 | 16       | 1.02          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD12 | 17       | 1.02          |
| (1,372) | 1:27:A:4PH:HE1  | 1:4:A:LYS:HG2   | 19       | 1.01          |
| (1,206) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG3   | 19       | 1.01          |
| (1,122) | 1:3:A:THR:HG23  | 1:4:A:LYS:H     | 2        | 1.01          |
| (1,77)  | 1:34:A:4PH:HD1  | 1:34:A:4PH:HA   | 15       | 1.01          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD11 | 2        | 1.01          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD13 | 5        | 1.01          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD12 | 8        | 1.01          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD11 | 12       | 1.01          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD13 | 14       | 1.01          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD13 | 18       | 1.01          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD13 | 19       | 1.01          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 8        | 1.01          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD12 | 1        | 1.0           |
| (1,32)  | 1:34:A:4PH:HB3  | 1:2:A:PRO:HG2   | 2        | 1.0           |
| (2,111) | 1:8:A:PRO:HD3   | 1:24:A:LEU:H    | 16       | 0.99          |
| (1,194) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HA   | 2        | 0.99          |
| (1,151) | 1:21:A:GLN:HE22 | 1:20:A:4PH:HD2  | 18       | 0.99          |
| (2,111) | 1:4:A:LYS:HA    | 1:24:A:LEU:H    | 6        | 0.98          |
| (2,110) | 1:27:A:4PH:HD2  | 1:5:A:PRO:HG2   | 1        | 0.98          |
| (2,85)  | 1:8:A:PRO:HD2   | 1:20:A:4PH:HD2  | 10       | 0.98          |
| (1,152) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG2   | 2        | 0.98          |
| (1,48)  | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD13 | 20       | 0.98          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33B | 14       | 0.98          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD23 | 14       | 0.98          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG3  | 7        | 0.97          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG2  | 10       | 0.97          |
| (2,62)  | 1:27:A:4PH:HD2  | 1:4:A:LYS:HG3   | 11       | 0.97          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 9        | 0.96          |
| (1,151) | 1:21:A:GLN:HE22 | 1:20:A:4PH:HD2  | 19       | 0.96          |
| (1,77)  | 1:34:A:4PH:HD1  | 1:34:A:4PH:HA   | 10       | 0.96          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33B | 8        | 0.96          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD23 | 13       | 0.96          |
| (2,103) | 1:4:A:LYS:H     | 1:27:A:4PH:HE2  | 9        | 0.95          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 12       | 0.95          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 3        | 0.95          |
| (1,194) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HA   | 1        | 0.95          |
| (1,122) | 1:3:A:THR:HG21  | 1:4:A:LYS:H     | 4        | 0.95          |
| (1,77)  | 1:34:A:4PH:HD1  | 1:34:A:4PH:HA   | 17       | 0.95          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 17       | 0.95          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33A | 3        | 0.95          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD23 | 10       | 0.95          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG3  | 9        | 0.94          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG3  | 17       | 0.94          |
| (2,62)  | 1:27:A:4PH:HD1  | 1:4:A:LYS:HG3   | 20       | 0.94          |
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 7        | 0.94          |
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 10       | 0.94          |
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 20       | 0.94          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 4        | 0.94          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 8        | 0.94          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 14       | 0.94          |
| (1,151) | 1:21:A:GLN:HE22 | 1:20:A:4PH:HD2  | 16       | 0.94          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33A | 19       | 0.94          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 7        | 0.93          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 17       | 0.93          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 18       | 0.93          |
| (1,77)  | 1:34:A:4PH:HD1  | 1:34:A:4PH:HA   | 14       | 0.93          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33A | 2        | 0.93          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33A | 5        | 0.93          |
| (2,41)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HB3   | 3        | 0.92          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 2        | 0.92          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 6        | 0.92          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 11       | 0.92          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 19       | 0.92          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 20       | 0.92          |
| (1,122) | 1:3:A:THR:HG23  | 1:4:A:LYS:H     | 15       | 0.92          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD21 | 13       | 0.92          |
| (1,77)  | 1:34:A:4PH:HD1  | 1:34:A:4PH:HA   | 4        | 0.92          |
| (2,91)  | 1:20:A:4PH:HB2  | 1:19:A:LYS:HG2  | 1        | 0.91          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 5        | 0.91          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 16       | 0.91          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 15       | 0.91          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD21 | 16       | 0.91          |
| (2,111) | 1:8:A:PRO:HD3   | 1:24:A:LEU:H    | 18       | 0.9           |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 14       | 0.9           |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 1        | 0.9           |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 10       | 0.9           |
| (1,122) | 1:3:A:THR:HG21  | 1:4:A:LYS:H     | 16       | 0.9           |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD22 | 12       | 0.9           |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 10       | 0.9           |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33B | 9        | 0.9           |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33A | 16       | 0.9           |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 8        | 0.89          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 13       | 0.89          |
| (1,77)  | 1:34:A:4PH:HD1  | 1:34:A:4PH:HA   | 13       | 0.89          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 12       | 0.88          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 12       | 0.88          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 13       | 0.88          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 16       | 0.88          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 2        | 0.88          |
| (1,152) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG2   | 20       | 0.87          |
| (1,122) | 1:3:A:THR:HG22  | 1:4:A:LYS:H     | 19       | 0.87          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD21 | 15       | 0.87          |
| (1,196) | 1:27:A:4PH:HD2  | 1:27:A:4PH:HA   | 15       | 0.86          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 3        | 0.86          |
| (1,140) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD3  | 18       | 0.86          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33B | 11       | 0.86          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD23 | 20       | 0.86          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 10       | 0.85          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 11       | 0.85          |
| (1,122) | 1:3:A:THR:HG22  | 1:4:A:LYS:H     | 14       | 0.85          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33A | 12       | 0.85          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H2    | 5        | 0.85          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33A | 4        | 0.84          |
| (2,111) | 1:4:A:LYS:HA    | 1:24:A:LEU:H    | 8        | 0.83          |
| (2,56)  | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD23 | 11       | 0.83          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 1        | 0.83          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 5        | 0.83          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,122) | 1:3:A:THR:HG22  | 1:4:A:LYS:H     | 8        | 0.83          |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD21 | 6        | 0.83          |
| (1,83)  | 1:20:A:4PH:HD2  | 1:20:A:4PH:HB2  | 14       | 0.83          |
| (1,83)  | 1:20:A:4PH:HD2  | 1:20:A:4PH:HB2  | 18       | 0.83          |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 14       | 0.83          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD21 | 3        | 0.83          |
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 18       | 0.82          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 11       | 0.82          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 14       | 0.82          |
| (1,83)  | 1:20:A:4PH:HD2  | 1:20:A:4PH:HB2  | 3        | 0.82          |
| (1,83)  | 1:20:A:4PH:HD2  | 1:20:A:4PH:HB2  | 11       | 0.82          |
| (1,83)  | 1:20:A:4PH:HD2  | 1:20:A:4PH:HB2  | 16       | 0.82          |
| (1,83)  | 1:20:A:4PH:HD2  | 1:20:A:4PH:HB2  | 19       | 0.82          |
| (1,83)  | 1:20:A:4PH:HD2  | 1:20:A:4PH:HB2  | 20       | 0.82          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD22 | 6        | 0.82          |
| (2,111) | 1:4:A:LYS:HA    | 1:24:A:LEU:H    | 1        | 0.81          |
| (2,13)  | 1:24:A:LEU:HD11 | 1:5:A:PRO:HG2   | 1        | 0.81          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 7        | 0.81          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 18       | 0.81          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 19       | 0.81          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 20       | 0.81          |
| (1,83)  | 1:20:A:4PH:HD2  | 1:20:A:4PH:HB2  | 1        | 0.81          |
| (1,83)  | 1:20:A:4PH:HD2  | 1:20:A:4PH:HB2  | 2        | 0.81          |
| (1,372) | 1:27:A:4PH:HE1  | 1:4:A:LYS:HG2   | 8        | 0.8           |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 17       | 0.8           |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 2        | 0.8           |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD22 | 15       | 0.8           |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD23 | 2        | 0.8           |
| (2,111) | 1:8:A:PRO:HD3   | 1:24:A:LEU:H    | 11       | 0.79          |
| (2,66)  | 1:20:A:4PH:HD1  | 1:24:A:LEU:HB3  | 19       | 0.79          |
| (2,66)  | 1:20:A:4PH:HD1  | 1:24:A:LEU:HB3  | 20       | 0.79          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 5        | 0.79          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 3        | 0.79          |
| (1,151) | 1:21:A:GLN:HE22 | 1:20:A:4PH:HD2  | 3        | 0.79          |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD23 | 15       | 0.79          |
| (1,52)  | 1:0:A:ACE:H2    | 1:1:A:PRO:HD2   | 6        | 0.79          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 18       | 0.78          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 4        | 0.78          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 8        | 0.78          |
| (1,122) | 1:3:A:THR:HG22  | 1:4:A:LYS:H     | 12       | 0.78          |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD23 | 9        | 0.78          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H3    | 4        | 0.78          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,66)  | 1:20:A:4PH:HD1  | 1:24:A:LEU:HB3  | 2        | 0.77          |
| (2,41)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HB3   | 6        | 0.77          |
| (1,372) | 1:27:A:4PH:HE1  | 1:4:A:LYS:HG2   | 11       | 0.77          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 1        | 0.77          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 6        | 0.77          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 17       | 0.77          |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD22 | 8        | 0.77          |
| (1,32)  | 1:34:A:4PH:HB3  | 1:2:A:PRO:HG2   | 19       | 0.77          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 10       | 0.76          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 7        | 0.76          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD22 | 19       | 0.76          |
| (2,55)  | 1:27:A:4PH:HD1  | 1:27:A:4PH:H33A | 1        | 0.75          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33B | 4        | 0.75          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33A | 6        | 0.75          |
| (2,55)  | 1:27:A:4PH:HD1  | 1:27:A:4PH:H33B | 7        | 0.75          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33  | 8        | 0.75          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33B | 9        | 0.75          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33  | 10       | 0.75          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33  | 11       | 0.75          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33B | 12       | 0.75          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33A | 13       | 0.75          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33A | 15       | 0.75          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33A | 17       | 0.75          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33  | 20       | 0.75          |
| (2,10)  | 1:7:A:LYS:HA    | 1:24:A:LEU:HD12 | 16       | 0.75          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 5        | 0.75          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 13       | 0.75          |
| (1,44)  | 1:31:A:LEU:HD12 | 1:31:A:LEU:HB2  | 20       | 0.75          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H2    | 6        | 0.75          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33B | 2        | 0.74          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33B | 3        | 0.74          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33B | 5        | 0.74          |
| (2,55)  | 1:27:A:4PH:HD1  | 1:27:A:4PH:H33B | 14       | 0.74          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33B | 16       | 0.74          |
| (2,55)  | 1:27:A:4PH:HD1  | 1:27:A:4PH:H33B | 18       | 0.74          |
| (2,41)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HB3   | 14       | 0.74          |
| (1,152) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG2   | 18       | 0.74          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H3    | 2        | 0.74          |
| (2,111) | 1:4:A:LYS:HA    | 1:24:A:LEU:H    | 17       | 0.73          |
| (2,55)  | 1:27:A:4PH:HD2  | 1:27:A:4PH:H33B | 19       | 0.73          |
| (1,152) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG2   | 19       | 0.73          |
| (1,122) | 1:3:A:THR:HG21  | 1:4:A:LYS:H     | 9        | 0.73          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,32)  | 1:34:A:4PH:HB3  | 1:2:A:PRO:HG2   | 6        | 0.73          |
| (1,372) | 1:27:A:4PH:HE1  | 1:4:A:LYS:HG2   | 5        | 0.72          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 15       | 0.72          |
| (1,44)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HB2  | 6        | 0.72          |
| (1,44)  | 1:31:A:LEU:HD11 | 1:31:A:LEU:HB2  | 16       | 0.72          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33  | 15       | 0.72          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H1    | 14       | 0.72          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 9        | 0.71          |
| (1,188) | 1:28:A:GLN:H    | 1:27:A:4PH:HD1  | 9        | 0.71          |
| (1,143) | 1:28:A:GLN:HG2  | 1:24:A:LEU:HD13 | 16       | 0.71          |
| (1,122) | 1:3:A:THR:HG23  | 1:4:A:LYS:H     | 6        | 0.71          |
| (1,44)  | 1:31:A:LEU:HD11 | 1:31:A:LEU:HB2  | 1        | 0.71          |
| (1,44)  | 1:31:A:LEU:HD11 | 1:31:A:LEU:HB2  | 2        | 0.71          |
| (1,44)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HB2  | 4        | 0.71          |
| (1,44)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HB2  | 8        | 0.71          |
| (1,44)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HB2  | 13       | 0.71          |
| (1,44)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HB2  | 14       | 0.71          |
| (1,44)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HB2  | 17       | 0.71          |
| (1,44)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HB2  | 19       | 0.71          |
| (1,372) | 1:27:A:4PH:HE1  | 1:4:A:LYS:HG2   | 13       | 0.7           |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 10       | 0.7           |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD23 | 20       | 0.7           |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD22 | 3        | 0.7           |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 3        | 0.7           |
| (1,44)  | 1:31:A:LEU:HD11 | 1:31:A:LEU:HB2  | 5        | 0.7           |
| (1,44)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HB2  | 9        | 0.7           |
| (1,44)  | 1:31:A:LEU:HD11 | 1:31:A:LEU:HB2  | 10       | 0.7           |
| (1,44)  | 1:31:A:LEU:HD11 | 1:31:A:LEU:HB2  | 15       | 0.7           |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 15       | 0.69          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 19       | 0.69          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 3        | 0.69          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 3        | 0.69          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 17       | 0.69          |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD21 | 10       | 0.69          |
| (1,44)  | 1:31:A:LEU:HD11 | 1:31:A:LEU:HB2  | 7        | 0.69          |
| (1,44)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HB2  | 11       | 0.69          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD22 | 9        | 0.69          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 4        | 0.68          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 7        | 0.68          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 14       | 0.68          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 9        | 0.68          |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD22 | 13       | 0.68          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG21  | 14       | 0.68          |
| (1,44)  | 1:31:A:LEU:HD13 | 1:31:A:LEU:HB2  | 3        | 0.68          |
| (2,56)  | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD21 | 16       | 0.67          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 11       | 0.67          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 17       | 0.67          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 2        | 0.67          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 8        | 0.67          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 9        | 0.67          |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 20       | 0.67          |
| (2,62)  | 1:27:A:4PH:HD2  | 1:4:A:LYS:HG3   | 1        | 0.66          |
| (1,372) | 1:27:A:4PH:HE1  | 1:4:A:LYS:HG2   | 3        | 0.66          |
| (1,372) | 1:27:A:4PH:HE1  | 1:4:A:LYS:HG2   | 7        | 0.66          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 16       | 0.66          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 18       | 0.66          |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG23  | 5        | 0.66          |
| (1,52)  | 1:0:A:ACE:H3    | 1:1:A:PRO:HD2   | 18       | 0.66          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 14       | 0.66          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 9        | 0.65          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 20       | 0.65          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 5        | 0.65          |
| (1,152) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG2   | 16       | 0.65          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB2  | 4        | 0.65          |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 4        | 0.65          |
| (2,41)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HB3   | 19       | 0.64          |
| (2,10)  | 1:7:A:LYS:HA    | 1:24:A:LEU:HD11 | 11       | 0.64          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 20       | 0.64          |
| (1,32)  | 1:34:A:4PH:HB3  | 1:2:A:PRO:HG2   | 4        | 0.64          |
| (2,66)  | 1:20:A:4PH:HD1  | 1:5:A:PRO:HG2   | 18       | 0.63          |
| (1,91)  | 1:27:A:4PH:HE1  | 1:2:A:PRO:HB3   | 6        | 0.63          |
| (1,52)  | 1:0:A:ACE:H3    | 1:1:A:PRO:HD2   | 9        | 0.63          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB2  | 3        | 0.63          |
| (2,66)  | 1:20:A:4PH:HD1  | 1:5:A:PRO:HG2   | 3        | 0.62          |
| (2,41)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HB3   | 20       | 0.62          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 7        | 0.62          |
| (1,296) | 1:31:A:LEU:HD23 | 1:27:A:4PH:H33A | 8        | 0.62          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 2        | 0.61          |
| (1,91)  | 1:27:A:4PH:HE1  | 1:2:A:PRO:HB3   | 16       | 0.61          |
| (1,52)  | 1:0:A:ACE:H3    | 1:1:A:PRO:HD2   | 3        | 0.61          |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB2  | 10       | 0.6           |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 16       | 0.6           |
| (1,197) | 1:27:A:4PH:HD1  | 1:27:A:4PH:HB2  | 2        | 0.6           |
| (1,197) | 1:27:A:4PH:HD1  | 1:27:A:4PH:HB2  | 3        | 0.6           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 5        | 0.6           |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 7        | 0.6           |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 8        | 0.6           |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 9        | 0.6           |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 10       | 0.6           |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 11       | 0.6           |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 14       | 0.6           |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 19       | 0.6           |
| (1,152) | 1:20:A:4PH:HE1 | 1:5:A:PRO:HG2  | 1        | 0.6           |
| (1,80)  | 1:27:A:4PH:HD1 | 1:24:A:LEU:HA  | 4        | 0.6           |
| (1,52)  | 1:0:A:ACE:H2   | 1:1:A:PRO:HD2  | 1        | 0.6           |
| (1,46)  | 1:5:A:PRO:HG2  | 1:4:A:LYS:HG3  | 11       | 0.6           |
| (1,372) | 1:27:A:4PH:HE1 | 1:4:A:LYS:HG2  | 2        | 0.59          |
| (1,313) | 1:25:A:ALA:HA  | 1:28:A:GLN:HB3 | 14       | 0.59          |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 4        | 0.59          |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 6        | 0.59          |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 13       | 0.59          |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 16       | 0.59          |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 17       | 0.59          |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 18       | 0.59          |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 20       | 0.59          |
| (1,80)  | 1:27:A:4PH:HD1 | 1:24:A:LEU:HA  | 2        | 0.59          |
| (1,52)  | 1:0:A:ACE:H1   | 1:1:A:PRO:HD2  | 8        | 0.59          |
| (2,42)  | 1:21:A:GLN:H   | 1:22:A:ALA:HB1 | 9        | 0.58          |
| (2,42)  | 1:21:A:GLN:H   | 1:22:A:ALA:HB3 | 13       | 0.58          |
| (2,36)  | 1:8:A:PRO:HD3  | 1:20:A:4PH:HD2 | 10       | 0.58          |
| (1,313) | 1:25:A:ALA:HA  | 1:28:A:GLN:HB3 | 19       | 0.58          |
| (1,267) | 1:26:A:LYS:HB3 | 1:23:A:ASP:HA  | 9        | 0.58          |
| (1,242) | 1:14:A:PRO:HD3 | 1:13:A:THR:HB  | 1        | 0.58          |
| (1,242) | 1:14:A:PRO:HD3 | 1:13:A:THR:HB  | 7        | 0.58          |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 1        | 0.58          |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 12       | 0.58          |
| (1,197) | 1:27:A:4PH:HD1 | 1:27:A:4PH:HB2 | 15       | 0.58          |
| (1,122) | 1:3:A:THR:HG21 | 1:4:A:LYS:H    | 13       | 0.58          |
| (1,35)  | 1:5:A:PRO:HD2  | 1:4:A:LYS:HG3  | 12       | 0.58          |
| (1,21)  | 1:34:A:4PH:HA  | 1:0:A:ACE:H3   | 15       | 0.58          |
| (2,42)  | 1:21:A:GLN:H   | 1:22:A:ALA:HB1 | 8        | 0.57          |
| (1,372) | 1:27:A:4PH:HE1 | 1:4:A:LYS:HG2  | 10       | 0.57          |
| (1,352) | 1:27:A:4PH:HE1 | 1:2:A:PRO:HG3  | 11       | 0.57          |
| (1,322) | 1:19:A:LYS:HG2 | 1:19:A:LYS:H   | 2        | 0.57          |
| (1,322) | 1:19:A:LYS:HG2 | 1:19:A:LYS:H   | 6        | 0.57          |
| (1,322) | 1:19:A:LYS:HG2 | 1:19:A:LYS:H   | 13       | 0.57          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 16       | 0.57          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 20       | 0.57          |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG22  | 3        | 0.57          |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG23  | 10       | 0.57          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB1  | 20       | 0.57          |
| (1,32)  | 1:34:A:4PH:HB3  | 1:2:A:PRO:HG2   | 3        | 0.57          |
| (2,66)  | 1:20:A:4PH:HD1  | 1:5:A:PRO:HG2   | 16       | 0.56          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 6        | 0.56          |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 5        | 0.56          |
| (1,52)  | 1:0:A:ACE:H1    | 1:1:A:PRO:HD2   | 15       | 0.56          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB2  | 7        | 0.56          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 1        | 0.56          |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB2  | 6        | 0.55          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 5        | 0.55          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 18       | 0.55          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 12       | 0.55          |
| (1,240) | 1:20:A:4PH:HD1  | 1:21:A:GLN:HE21 | 19       | 0.55          |
| (1,152) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG2   | 14       | 0.55          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB1  | 2        | 0.55          |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB1  | 1        | 0.54          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 11       | 0.54          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 2        | 0.54          |
| (1,117) | 1:28:A:GLN:HE21 | 1:24:A:LEU:HD23 | 2        | 0.54          |
| (1,52)  | 1:0:A:ACE:H1    | 1:1:A:PRO:HD2   | 12       | 0.54          |
| (1,52)  | 1:0:A:ACE:H1    | 1:1:A:PRO:HD2   | 20       | 0.54          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB1  | 11       | 0.54          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H1    | 8        | 0.54          |
| (2,50)  | 1:27:A:4PH:HD2  | 1:31:A:LEU:HD23 | 18       | 0.53          |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB2  | 5        | 0.53          |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB2  | 14       | 0.53          |
| (1,373) | 1:27:A:4PH:HD2  | 1:4:A:LYS:HA    | 15       | 0.53          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 8        | 0.53          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 20       | 0.53          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 3        | 0.53          |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG21  | 11       | 0.53          |
| (1,91)  | 1:27:A:4PH:HE1  | 1:2:A:PRO:HB3   | 19       | 0.53          |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 11       | 0.53          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 17       | 0.52          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 2        | 0.52          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 6        | 0.52          |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG21  | 4        | 0.52          |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB1  | 19       | 0.51          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,13)  | 1:24:A:LEU:HD11 | 1:5:A:PRO:HG2   | 14       | 0.51          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 12       | 0.51          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 6        | 0.51          |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 3        | 0.51          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB1  | 5        | 0.51          |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB3  | 2        | 0.5           |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB1  | 7        | 0.5           |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB3  | 12       | 0.5           |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB1  | 17       | 0.5           |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 3        | 0.5           |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 1        | 0.5           |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 14       | 0.5           |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 20       | 0.5           |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 5        | 0.5           |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 8        | 0.5           |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 18       | 0.5           |
| (1,52)  | 1:0:A:ACE:H2    | 1:1:A:PRO:HD2   | 16       | 0.5           |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33  | 13       | 0.5           |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB1  | 11       | 0.49          |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB3  | 15       | 0.49          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 12       | 0.49          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 10       | 0.49          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 3        | 0.49          |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 8        | 0.49          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB1  | 16       | 0.49          |
| (1,46)  | 1:5:A:PRO:HG2   | 1:4:A:LYS:HG3   | 19       | 0.49          |
| (1,32)  | 1:34:A:4PH:HB3  | 1:2:A:PRO:HG2   | 9        | 0.49          |
| (1,32)  | 1:34:A:4PH:HB3  | 1:2:A:PRO:HG2   | 15       | 0.49          |
| (1,32)  | 1:34:A:4PH:HB3  | 1:2:A:PRO:HG2   | 17       | 0.49          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H3    | 10       | 0.49          |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB3  | 20       | 0.48          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 10       | 0.48          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 19       | 0.48          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 4        | 0.48          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 19       | 0.48          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 8        | 0.48          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 13       | 0.48          |
| (1,152) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG2   | 11       | 0.48          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 16       | 0.48          |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 9        | 0.48          |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB2  | 18       | 0.47          |
| (1,322) | 1:19:A:LYS:HG2  | 1:19:A:LYS:H    | 1        | 0.47          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 8        | 0.47          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 13       | 0.47          |
| (1,240) | 1:20:A:4PH:HD1  | 1:21:A:GLN:HE21 | 3        | 0.47          |
| (1,240) | 1:20:A:4PH:HD2  | 1:21:A:GLN:HE21 | 10       | 0.47          |
| (1,93)  | 1:34:A:4PH:HD1  | 1:0:A:ACE:H1    | 7        | 0.47          |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 6        | 0.47          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB3  | 15       | 0.47          |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB2  | 3        | 0.46          |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB3  | 4        | 0.46          |
| (2,42)  | 1:21:A:GLN:H    | 1:22:A:ALA:HB1  | 16       | 0.46          |
| (2,17)  | 1:20:A:4PH:H33A | 1:7:A:LYS:HE2   | 13       | 0.46          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 16       | 0.46          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 10       | 0.46          |
| (1,240) | 1:20:A:4PH:HD2  | 1:21:A:GLN:HE21 | 4        | 0.46          |
| (1,112) | 1:20:A:4PH:HD1  | 1:17:A:LEU:HD22 | 18       | 0.46          |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG23  | 9        | 0.46          |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 19       | 0.46          |
| (2,13)  | 1:24:A:LEU:HD12 | 1:5:A:PRO:HG2   | 8        | 0.45          |
| (2,13)  | 1:24:A:LEU:HD13 | 1:5:A:PRO:HG2   | 17       | 0.45          |
| (1,372) | 1:27:A:4PH:HE1  | 1:4:A:LYS:HG2   | 14       | 0.45          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 4        | 0.45          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 18       | 0.45          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 2        | 0.45          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 5        | 0.45          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 6        | 0.45          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 9        | 0.45          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 12       | 0.45          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 13       | 0.45          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 14       | 0.45          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 15       | 0.45          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 17       | 0.45          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 19       | 0.45          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 20       | 0.45          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 4        | 0.45          |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 17       | 0.45          |
| (2,99)  | 1:27:A:4PH:H    | 1:26:A:LYS:HG3  | 5        | 0.44          |
| (2,66)  | 1:20:A:4PH:HD1  | 1:5:A:PRO:HG2   | 14       | 0.44          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 4        | 0.44          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 7        | 0.44          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 8        | 0.44          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 10       | 0.44          |
| (1,308) | 1:15:A:GLU:HG3  | 1:15:A:GLU:HB3  | 11       | 0.44          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,308) | 1:15:A:GLU:HG3 | 1:15:A:GLU:HB3  | 16       | 0.44          |
| (1,308) | 1:15:A:GLU:HG3 | 1:15:A:GLU:HB3  | 18       | 0.44          |
| (1,242) | 1:14:A:PRO:HD3 | 1:13:A:THR:HB   | 17       | 0.44          |
| (1,112) | 1:20:A:4PH:HD2 | 1:17:A:LEU:HD22 | 10       | 0.44          |
| (1,80)  | 1:27:A:4PH:HD1 | 1:24:A:LEU:HA   | 7        | 0.44          |
| (1,80)  | 1:27:A:4PH:HD1 | 1:24:A:LEU:HA   | 13       | 0.44          |
| (1,80)  | 1:27:A:4PH:HD1 | 1:24:A:LEU:HA   | 20       | 0.44          |
| (2,66)  | 1:20:A:4PH:HD1 | 1:5:A:PRO:HG2   | 11       | 0.43          |
| (1,313) | 1:25:A:ALA:HA  | 1:28:A:GLN:HB3  | 1        | 0.43          |
| (1,308) | 1:15:A:GLU:HG3 | 1:15:A:GLU:HB3  | 3        | 0.43          |
| (1,297) | 1:21:A:GLN:HA  | 1:24:A:LEU:HB3  | 4        | 0.43          |
| (1,240) | 1:20:A:4PH:HD2 | 1:21:A:GLN:HE21 | 8        | 0.43          |
| (1,116) | 1:20:A:4PH:HE2 | 1:24:A:LEU:HD23 | 12       | 0.43          |
| (1,112) | 1:20:A:4PH:HD2 | 1:17:A:LEU:HD21 | 13       | 0.43          |
| (1,32)  | 1:34:A:4PH:HB3 | 1:2:A:PRO:HG2   | 12       | 0.43          |
| (1,32)  | 1:34:A:4PH:HB3 | 1:2:A:PRO:HG2   | 16       | 0.43          |
| (2,28)  | 1:27:A:4PH:HD1 | 1:5:A:PRO:HD3   | 1        | 0.42          |
| (1,297) | 1:21:A:GLN:HA  | 1:24:A:LEU:HB3  | 6        | 0.42          |
| (1,209) | 1:20:A:4PH:HE1 | 1:7:A:LYS:HA    | 20       | 0.42          |
| (1,112) | 1:20:A:4PH:HD2 | 1:17:A:LEU:HD21 | 12       | 0.42          |
| (1,74)  | 1:3:A:THR:HA   | 1:27:A:4PH:HE1  | 10       | 0.42          |
| (1,49)  | 1:8:A:PRO:HB3  | 1:12:A:ALA:HB2  | 1        | 0.42          |
| (1,49)  | 1:8:A:PRO:HB3  | 1:12:A:ALA:HB2  | 17       | 0.42          |
| (1,49)  | 1:8:A:PRO:HB3  | 1:12:A:ALA:HB2  | 19       | 0.42          |
| (1,239) | 1:34:A:4PH:HB2 | 1:34:A:4PH:HD2  | 2        | 0.41          |
| (1,239) | 1:34:A:4PH:HB2 | 1:34:A:4PH:HD2  | 5        | 0.41          |
| (1,239) | 1:34:A:4PH:HB2 | 1:34:A:4PH:HD2  | 11       | 0.41          |
| (1,239) | 1:34:A:4PH:HB2 | 1:34:A:4PH:HD2  | 15       | 0.41          |
| (1,116) | 1:20:A:4PH:HE2 | 1:24:A:LEU:HD22 | 6        | 0.41          |
| (1,91)  | 1:27:A:4PH:HE1 | 1:2:A:PRO:HB3   | 13       | 0.41          |
| (1,80)  | 1:27:A:4PH:HD1 | 1:24:A:LEU:HA   | 12       | 0.41          |
| (1,35)  | 1:5:A:PRO:HD2  | 1:4:A:LYS:HG3   | 6        | 0.41          |
| (1,35)  | 1:5:A:PRO:HD2  | 1:4:A:LYS:HG3   | 15       | 0.41          |
| (2,85)  | 1:8:A:PRO:HD2  | 1:20:A:4PH:HD1  | 20       | 0.4           |
| (1,373) | 1:27:A:4PH:HD2 | 1:4:A:LYS:HA    | 1        | 0.4           |
| (1,372) | 1:27:A:4PH:HE1 | 1:4:A:LYS:HG2   | 15       | 0.4           |
| (1,352) | 1:27:A:4PH:HE1 | 1:2:A:PRO:HG3   | 5        | 0.4           |
| (1,345) | 1:8:A:PRO:HB3  | 1:8:A:PRO:HD2   | 1        | 0.4           |
| (1,345) | 1:8:A:PRO:HB3  | 1:8:A:PRO:HD2   | 5        | 0.4           |
| (1,345) | 1:8:A:PRO:HB3  | 1:8:A:PRO:HD2   | 6        | 0.4           |
| (1,345) | 1:8:A:PRO:HB3  | 1:8:A:PRO:HD2   | 8        | 0.4           |
| (1,345) | 1:8:A:PRO:HB3  | 1:8:A:PRO:HD2   | 12       | 0.4           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 18       | 0.4           |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 15       | 0.4           |
| (1,240) | 1:20:A:4PH:HD2  | 1:21:A:GLN:HE21 | 7        | 0.4           |
| (1,239) | 1:34:A:4PH:HB2  | 1:34:A:4PH:HD2  | 4        | 0.4           |
| (1,239) | 1:34:A:4PH:HB2  | 1:34:A:4PH:HD2  | 10       | 0.4           |
| (1,372) | 1:27:A:4PH:HE1  | 1:4:A:LYS:HG2   | 12       | 0.39          |
| (1,372) | 1:27:A:4PH:HE1  | 1:4:A:LYS:HG2   | 16       | 0.39          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 9        | 0.39          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 13       | 0.39          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 15       | 0.39          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 16       | 0.39          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 19       | 0.39          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 20       | 0.39          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 19       | 0.39          |
| (1,240) | 1:20:A:4PH:HD1  | 1:21:A:GLN:HE21 | 2        | 0.39          |
| (1,239) | 1:34:A:4PH:HB2  | 1:34:A:4PH:HD2  | 14       | 0.39          |
| (1,239) | 1:34:A:4PH:HB2  | 1:34:A:4PH:HD2  | 17       | 0.39          |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 16       | 0.39          |
| (2,41)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HB3   | 11       | 0.38          |
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 13       | 0.38          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 2        | 0.38          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 3        | 0.38          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 4        | 0.38          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 10       | 0.38          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 11       | 0.38          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 17       | 0.38          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 5        | 0.38          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 15       | 0.38          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 11       | 0.38          |
| (1,239) | 1:34:A:4PH:HB2  | 1:34:A:4PH:HD2  | 13       | 0.38          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 5        | 0.38          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 11       | 0.38          |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD23 | 8        | 0.38          |
| (1,91)  | 1:27:A:4PH:HE1  | 1:2:A:PRO:HB3   | 11       | 0.38          |
| (1,74)  | 1:3:A:THR:HA    | 1:27:A:4PH:HE1  | 2        | 0.38          |
| (1,52)  | 1:0:A:ACE:H1    | 1:1:A:PRO:HD2   | 11       | 0.38          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB1  | 9        | 0.38          |
| (2,13)  | 1:24:A:LEU:HD13 | 1:5:A:PRO:HG2   | 6        | 0.37          |
| (1,364) | 1:0:A:ACE:H3    | 1:34:A:4PH:HB3  | 11       | 0.37          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 7        | 0.37          |
| (1,345) | 1:8:A:PRO:HB3   | 1:8:A:PRO:HD2   | 14       | 0.37          |
| (1,257) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3  | 18       | 0.37          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,240) | 1:20:A:4PH:HD1  | 1:21:A:GLN:HE21 | 14       | 0.37          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 16       | 0.37          |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 12       | 0.37          |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 15       | 0.37          |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 16       | 0.37          |
| (1,91)  | 1:27:A:4PH:HE1  | 1:2:A:PRO:HB3   | 12       | 0.37          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33B | 20       | 0.37          |
| (1,34)  | 1:5:A:PRO:HD2   | 1:24:A:LEU:HD13 | 10       | 0.37          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD22 | 17       | 0.37          |
| (2,71)  | 1:34:A:4PH:H    | 1:34:A:4PH:HD2  | 4        | 0.36          |
| (2,41)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HB3   | 10       | 0.36          |
| (2,13)  | 1:24:A:LEU:HD12 | 1:5:A:PRO:HG2   | 18       | 0.36          |
| (1,372) | 1:27:A:4PH:HE1  | 1:4:A:LYS:HG2   | 4        | 0.36          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 16       | 0.36          |
| (1,257) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3  | 7        | 0.36          |
| (1,257) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3  | 8        | 0.36          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 3        | 0.36          |
| (1,240) | 1:20:A:4PH:HD2  | 1:21:A:GLN:HE21 | 6        | 0.36          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 6        | 0.36          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 9        | 0.36          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 17       | 0.36          |
| (1,152) | 1:20:A:4PH:HE1  | 1:5:A:PRO:HG2   | 3        | 0.36          |
| (1,112) | 1:20:A:4PH:HD1  | 1:17:A:LEU:HD23 | 1        | 0.36          |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG21  | 2        | 0.36          |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 10       | 0.36          |
| (1,52)  | 1:0:A:ACE:H3    | 1:1:A:PRO:HD2   | 5        | 0.36          |
| (1,52)  | 1:0:A:ACE:H3    | 1:1:A:PRO:HD2   | 19       | 0.36          |
| (1,32)  | 1:34:A:4PH:HB3  | 1:2:A:PRO:HG2   | 13       | 0.36          |
| (2,71)  | 1:20:A:4PH:H    | 1:20:A:4PH:HD1  | 17       | 0.35          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 13       | 0.35          |
| (1,257) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3  | 3        | 0.35          |
| (1,257) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3  | 14       | 0.35          |
| (1,257) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3  | 17       | 0.35          |
| (1,257) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3  | 20       | 0.35          |
| (1,240) | 1:20:A:4PH:HD1  | 1:21:A:GLN:HE21 | 1        | 0.35          |
| (1,240) | 1:20:A:4PH:HD2  | 1:21:A:GLN:HE21 | 12       | 0.35          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 4        | 0.35          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 8        | 0.35          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 10       | 0.35          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 12       | 0.35          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 13       | 0.35          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 14       | 0.35          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 15       | 0.35          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 20       | 0.35          |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 10       | 0.35          |
| (1,112) | 1:20:A:4PH:HD1  | 1:17:A:LEU:HD21 | 14       | 0.35          |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG23  | 13       | 0.35          |
| (1,51)  | 1:0:A:ACE:H3    | 1:1:A:PRO:HD3   | 7        | 0.35          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB2  | 6        | 0.35          |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 13       | 0.35          |
| (2,36)  | 1:8:A:PRO:HD3   | 1:20:A:4PH:HD2  | 2        | 0.34          |
| (1,296) | 1:31:A:LEU:HD21 | 1:27:A:4PH:H33A | 11       | 0.34          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 14       | 0.34          |
| (1,257) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3  | 1        | 0.34          |
| (1,257) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3  | 6        | 0.34          |
| (1,257) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3  | 9        | 0.34          |
| (1,257) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3  | 19       | 0.34          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 12       | 0.34          |
| (1,240) | 1:20:A:4PH:HD2  | 1:21:A:GLN:HE21 | 9        | 0.34          |
| (1,240) | 1:20:A:4PH:HD2  | 1:21:A:GLN:HE21 | 17       | 0.34          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 2        | 0.34          |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG22  | 16       | 0.34          |
| (1,93)  | 1:34:A:4PH:HD2  | 1:0:A:ACE:H3    | 13       | 0.34          |
| (2,71)  | 1:34:A:4PH:H    | 1:34:A:4PH:HD1  | 1        | 0.33          |
| (2,71)  | 1:34:A:4PH:H    | 1:34:A:4PH:HD2  | 2        | 0.33          |
| (2,71)  | 1:34:A:4PH:H    | 1:34:A:4PH:HD1  | 7        | 0.33          |
| (2,71)  | 1:34:A:4PH:H    | 1:34:A:4PH:HD2  | 15       | 0.33          |
| (1,296) | 1:31:A:LEU:HD22 | 1:27:A:4PH:H33A | 20       | 0.33          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 11       | 0.33          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 18       | 0.33          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 20       | 0.33          |
| (1,257) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3  | 4        | 0.33          |
| (1,240) | 1:20:A:4PH:HD2  | 1:21:A:GLN:HE21 | 15       | 0.33          |
| (1,240) | 1:20:A:4PH:HD1  | 1:21:A:GLN:HE21 | 18       | 0.33          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 1        | 0.33          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 3        | 0.33          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 7        | 0.33          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 18       | 0.33          |
| (1,219) | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 19       | 0.33          |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB1  | 18       | 0.33          |
| (1,52)  | 1:0:A:ACE:H1    | 1:1:A:PRO:HD2   | 4        | 0.33          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB2  | 18       | 0.33          |
| (2,71)  | 1:34:A:4PH:H    | 1:34:A:4PH:HD2  | 5        | 0.32          |
| (2,71)  | 1:20:A:4PH:H    | 1:20:A:4PH:HD2  | 8        | 0.32          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,71)  | 1:20:A:4PH:H    | 1:20:A:4PH:HD1  | 10       | 0.32          |
| (2,71)  | 1:20:A:4PH:H    | 1:20:A:4PH:HD1  | 18       | 0.32          |
| (1,296) | 1:31:A:LEU:HD21 | 1:27:A:4PH:H33  | 9        | 0.32          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 2        | 0.32          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 3        | 0.32          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 4        | 0.32          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 6        | 0.32          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 7        | 0.32          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 8        | 0.32          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 16       | 0.32          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 17       | 0.32          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 19       | 0.32          |
| (1,257) | 1:24:A:LEU:HD23 | 1:24:A:LEU:HB3  | 2        | 0.32          |
| (1,257) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3  | 13       | 0.32          |
| (1,257) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3  | 15       | 0.32          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 15       | 0.32          |
| (1,242) | 1:14:A:PRO:HD3  | 1:13:A:THR:HB   | 18       | 0.32          |
| (1,240) | 1:20:A:4PH:HD2  | 1:21:A:GLN:HE21 | 5        | 0.32          |
| (1,139) | 1:15:A:GLU:HG3  | 1:14:A:PRO:HD2  | 1        | 0.32          |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 7        | 0.32          |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG21  | 17       | 0.32          |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB3  | 16       | 0.32          |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 1        | 0.32          |
| (1,52)  | 1:0:A:ACE:H1    | 1:1:A:PRO:HD2   | 2        | 0.32          |
| (2,74)  | 1:20:A:4PH:HD1  | 1:20:A:4PH:HB3  | 2        | 0.31          |
| (2,71)  | 1:34:A:4PH:H    | 1:34:A:4PH:HD1  | 9        | 0.31          |
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 1        | 0.31          |
| (1,297) | 1:21:A:GLN:HA   | 1:24:A:LEU:HB3  | 9        | 0.31          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 9        | 0.31          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 10       | 0.31          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 13       | 0.31          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 15       | 0.31          |
| (1,257) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3  | 5        | 0.31          |
| (1,257) | 1:24:A:LEU:HD21 | 1:24:A:LEU:HB3  | 10       | 0.31          |
| (1,257) | 1:24:A:LEU:HD22 | 1:24:A:LEU:HB3  | 12       | 0.31          |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD12 | 14       | 0.31          |
| (1,195) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HB3  | 1        | 0.31          |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB3  | 2        | 0.31          |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB1  | 19       | 0.31          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB1  | 14       | 0.31          |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 7        | 0.31          |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 8        | 0.31          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,74)  | 1:20:A:4PH:HD1  | 1:20:A:4PH:HB3  | 11       | 0.3           |
| (2,71)  | 1:20:A:4PH:H    | 1:20:A:4PH:HD2  | 20       | 0.3           |
| (2,41)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HB3   | 15       | 0.3           |
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 4        | 0.3           |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 12       | 0.3           |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD12 | 3        | 0.3           |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD12 | 8        | 0.3           |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD12 | 9        | 0.3           |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD13 | 10       | 0.3           |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 11       | 0.3           |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD23 | 5        | 0.3           |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB1  | 1        | 0.3           |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB3  | 11       | 0.3           |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB2  | 15       | 0.3           |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB1  | 8        | 0.3           |
| (2,38)  | 1:27:A:4PH:HE2  | 1:27:A:4PH:H33A | 6        | 0.29          |
| (2,38)  | 1:27:A:4PH:HE2  | 1:27:A:4PH:H33  | 7        | 0.29          |
| (2,38)  | 1:27:A:4PH:HE2  | 1:27:A:4PH:H33  | 8        | 0.29          |
| (2,38)  | 1:27:A:4PH:HE1  | 1:27:A:4PH:H33B | 10       | 0.29          |
| (2,38)  | 1:27:A:4PH:HE2  | 1:27:A:4PH:H33  | 11       | 0.29          |
| (2,38)  | 1:27:A:4PH:HE2  | 1:27:A:4PH:H33B | 12       | 0.29          |
| (2,38)  | 1:27:A:4PH:HE2  | 1:27:A:4PH:H33A | 13       | 0.29          |
| (2,38)  | 1:27:A:4PH:HE1  | 1:27:A:4PH:H33B | 14       | 0.29          |
| (2,38)  | 1:27:A:4PH:HE2  | 1:27:A:4PH:H33A | 15       | 0.29          |
| (2,38)  | 1:27:A:4PH:HE2  | 1:27:A:4PH:H33B | 16       | 0.29          |
| (2,38)  | 1:27:A:4PH:HE1  | 1:27:A:4PH:H33  | 17       | 0.29          |
| (2,38)  | 1:27:A:4PH:HE1  | 1:27:A:4PH:H33  | 19       | 0.29          |
| (2,38)  | 1:27:A:4PH:HE1  | 1:27:A:4PH:H33B | 20       | 0.29          |
| (2,34)  | 1:5:A:PRO:HD2   | 1:27:A:4PH:HD2  | 1        | 0.29          |
| (1,313) | 1:25:A:ALA:HA   | 1:28:A:GLN:HB3  | 11       | 0.29          |
| (1,296) | 1:31:A:LEU:HD21 | 1:27:A:4PH:H33B | 6        | 0.29          |
| (1,264) | 1:26:A:LYS:H    | 1:26:A:LYS:HB3  | 1        | 0.29          |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD13 | 2        | 0.29          |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD13 | 5        | 0.29          |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD12 | 11       | 0.29          |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD12 | 13       | 0.29          |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD12 | 17       | 0.29          |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD12 | 19       | 0.29          |
| (1,195) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HB3  | 2        | 0.29          |
| (1,195) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HB3  | 16       | 0.29          |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD22 | 14       | 0.29          |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB1  | 4        | 0.29          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,107) | 1:13:A:THR:H   | 1:12:A:ALA:HB1  | 7        | 0.29          |
| (1,107) | 1:13:A:THR:H   | 1:12:A:ALA:HB2  | 12       | 0.29          |
| (1,107) | 1:13:A:THR:H   | 1:12:A:ALA:HB3  | 20       | 0.29          |
| (1,91)  | 1:27:A:4PH:HE1 | 1:2:A:PRO:HB3   | 4        | 0.29          |
| (1,52)  | 1:0:A:ACE:H1   | 1:1:A:PRO:HD2   | 10       | 0.29          |
| (1,52)  | 1:0:A:ACE:H1   | 1:1:A:PRO:HD2   | 13       | 0.29          |
| (2,71)  | 1:34:A:4PH:H   | 1:34:A:4PH:HD1  | 3        | 0.28          |
| (2,71)  | 1:20:A:4PH:H   | 1:20:A:4PH:HD2  | 6        | 0.28          |
| (2,71)  | 1:34:A:4PH:H   | 1:34:A:4PH:HD1  | 12       | 0.28          |
| (2,38)  | 1:27:A:4PH:HE1 | 1:27:A:4PH:H33A | 1        | 0.28          |
| (2,38)  | 1:27:A:4PH:HE2 | 1:27:A:4PH:H33B | 2        | 0.28          |
| (2,38)  | 1:27:A:4PH:HE2 | 1:27:A:4PH:H33B | 3        | 0.28          |
| (2,38)  | 1:27:A:4PH:HE2 | 1:27:A:4PH:H33B | 4        | 0.28          |
| (2,38)  | 1:27:A:4PH:HE2 | 1:27:A:4PH:H33B | 5        | 0.28          |
| (2,38)  | 1:27:A:4PH:HE2 | 1:27:A:4PH:H33B | 9        | 0.28          |
| (2,38)  | 1:27:A:4PH:HE1 | 1:27:A:4PH:H33B | 18       | 0.28          |
| (1,264) | 1:26:A:LYS:H   | 1:26:A:LYS:HB3  | 5        | 0.28          |
| (1,212) | 1:31:A:LEU:H   | 1:31:A:LEU:HD13 | 1        | 0.28          |
| (1,212) | 1:31:A:LEU:H   | 1:31:A:LEU:HD12 | 4        | 0.28          |
| (1,212) | 1:31:A:LEU:H   | 1:31:A:LEU:HD13 | 7        | 0.28          |
| (1,212) | 1:31:A:LEU:H   | 1:31:A:LEU:HD13 | 15       | 0.28          |
| (1,212) | 1:31:A:LEU:H   | 1:31:A:LEU:HD13 | 16       | 0.28          |
| (1,195) | 1:20:A:4PH:HD1 | 1:20:A:4PH:HB3  | 11       | 0.28          |
| (1,138) | 1:28:A:GLN:HA  | 1:27:A:4PH:HD1  | 1        | 0.28          |
| (1,138) | 1:28:A:GLN:HA  | 1:27:A:4PH:HD1  | 13       | 0.28          |
| (1,116) | 1:20:A:4PH:HE2 | 1:24:A:LEU:HD22 | 10       | 0.28          |
| (1,107) | 1:13:A:THR:H   | 1:12:A:ALA:HB3  | 9        | 0.28          |
| (1,91)  | 1:27:A:4PH:HE1 | 1:2:A:PRO:HB3   | 17       | 0.28          |
| (1,52)  | 1:0:A:ACE:H3   | 1:1:A:PRO:HD2   | 17       | 0.28          |
| (1,49)  | 1:8:A:PRO:HB3  | 1:12:A:ALA:HB1  | 13       | 0.28          |
| (2,74)  | 1:20:A:4PH:HD1 | 1:20:A:4PH:HB3  | 14       | 0.27          |
| (2,66)  | 1:20:A:4PH:HD1 | 1:5:A:PRO:HG2   | 1        | 0.27          |
| (2,41)  | 1:34:A:4PH:HE1 | 1:1:A:PRO:HB3   | 7        | 0.27          |
| (1,352) | 1:27:A:4PH:HE1 | 1:2:A:PRO:HG3   | 14       | 0.27          |
| (1,352) | 1:27:A:4PH:HE1 | 1:2:A:PRO:HG3   | 19       | 0.27          |
| (1,343) | 1:4:A:LYS:HB2  | 1:4:A:LYS:H     | 6        | 0.27          |
| (1,240) | 1:20:A:4PH:HD1 | 1:21:A:GLN:HE21 | 11       | 0.27          |
| (1,212) | 1:31:A:LEU:H   | 1:31:A:LEU:HD12 | 6        | 0.27          |
| (1,195) | 1:20:A:4PH:HD1 | 1:20:A:4PH:HB3  | 19       | 0.27          |
| (1,138) | 1:28:A:GLN:HA  | 1:27:A:4PH:HD1  | 4        | 0.27          |
| (1,124) | 1:11:A:ASN:HB3 | 1:11:A:ASN:HD22 | 11       | 0.27          |
| (1,107) | 1:13:A:THR:H   | 1:12:A:ALA:HB1  | 3        | 0.27          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB1  | 6        | 0.27          |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB3  | 13       | 0.27          |
| (1,91)  | 1:27:A:4PH:HE1  | 1:2:A:PRO:HB3   | 3        | 0.27          |
| (1,91)  | 1:27:A:4PH:HE1  | 1:2:A:PRO:HB3   | 9        | 0.27          |
| (1,74)  | 1:3:A:THR:HA    | 1:27:A:4PH:HE1  | 5        | 0.27          |
| (1,49)  | 1:8:A:PRO:HB3   | 1:12:A:ALA:HB3  | 12       | 0.27          |
| (1,43)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HD13 | 10       | 0.27          |
| (2,71)  | 1:20:A:4PH:H    | 1:20:A:4PH:HD1  | 11       | 0.26          |
| (2,71)  | 1:20:A:4PH:H    | 1:20:A:4PH:HD1  | 13       | 0.26          |
| (2,71)  | 1:34:A:4PH:H    | 1:34:A:4PH:HD1  | 19       | 0.26          |
| (2,27)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HA    | 11       | 0.26          |
| (1,267) | 1:26:A:LYS:HB3  | 1:23:A:ASP:HA   | 7        | 0.26          |
| (1,212) | 1:31:A:LEU:H    | 1:31:A:LEU:HD11 | 20       | 0.26          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 1        | 0.26          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 7        | 0.26          |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD22 | 17       | 0.26          |
| (1,91)  | 1:27:A:4PH:HE1  | 1:2:A:PRO:HB3   | 15       | 0.26          |
| (1,43)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HD12 | 1        | 0.26          |
| (1,43)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HD12 | 5        | 0.26          |
| (1,43)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HD13 | 7        | 0.26          |
| (1,43)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HD12 | 11       | 0.26          |
| (1,43)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HD11 | 13       | 0.26          |
| (1,43)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HD11 | 17       | 0.26          |
| (1,43)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HD11 | 19       | 0.26          |
| (2,39)  | 1:20:A:4PH:HE2  | 1:20:A:4PH:H33  | 6        | 0.25          |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33A | 7        | 0.25          |
| (2,39)  | 1:20:A:4PH:HE2  | 1:20:A:4PH:H33A | 13       | 0.25          |
| (2,39)  | 1:20:A:4PH:HE2  | 1:20:A:4PH:H33A | 20       | 0.25          |
| (2,20)  | 1:18:A:ALA:HB3  | 1:15:A:GLU:HA   | 7        | 0.25          |
| (1,364) | 1:0:A:ACE:H3    | 1:34:A:4PH:HB3  | 13       | 0.25          |
| (1,296) | 1:31:A:LEU:HD22 | 1:27:A:4PH:H33B | 13       | 0.25          |
| (1,195) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HB3  | 3        | 0.25          |
| (1,195) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HB3  | 14       | 0.25          |
| (1,195) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HB3  | 18       | 0.25          |
| (1,195) | 1:20:A:4PH:HD1  | 1:20:A:4PH:HB3  | 20       | 0.25          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 2        | 0.25          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 6        | 0.25          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 9        | 0.25          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 10       | 0.25          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 17       | 0.25          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 18       | 0.25          |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD21 | 20       | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG21  | 19       | 0.25          |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB1  | 10       | 0.25          |
| (1,43)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HD12 | 2        | 0.25          |
| (1,43)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HD12 | 3        | 0.25          |
| (1,43)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HD11 | 4        | 0.25          |
| (1,43)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HD11 | 9        | 0.25          |
| (1,43)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HD12 | 15       | 0.25          |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 17       | 0.25          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H3    | 20       | 0.25          |
| (1,18)  | 1:28:A:GLN:HA   | 1:31:A:LEU:HD22 | 1        | 0.25          |
| (2,71)  | 1:34:A:4PH:H    | 1:34:A:4PH:HD2  | 14       | 0.24          |
| (2,39)  | 1:20:A:4PH:HE2  | 1:20:A:4PH:H33B | 4        | 0.24          |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33  | 5        | 0.24          |
| (2,39)  | 1:20:A:4PH:HE2  | 1:20:A:4PH:H33B | 8        | 0.24          |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33  | 10       | 0.24          |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33B | 12       | 0.24          |
| (2,39)  | 1:20:A:4PH:HE2  | 1:20:A:4PH:H33B | 15       | 0.24          |
| (2,39)  | 1:20:A:4PH:HE2  | 1:20:A:4PH:H33A | 17       | 0.24          |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33A | 18       | 0.24          |
| (1,364) | 1:0:A:ACE:H2    | 1:34:A:4PH:HB3  | 3        | 0.24          |
| (1,296) | 1:31:A:LEU:HD21 | 1:27:A:4PH:H33  | 4        | 0.24          |
| (1,266) | 1:26:A:LYS:HG2  | 1:26:A:LYS:H    | 20       | 0.24          |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 5        | 0.24          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 4        | 0.24          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 12       | 0.24          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 13       | 0.24          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 14       | 0.24          |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB3  | 5        | 0.24          |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB1  | 17       | 0.24          |
| (1,93)  | 1:34:A:4PH:HD1  | 1:0:A:ACE:H3    | 19       | 0.24          |
| (1,43)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HD11 | 6        | 0.24          |
| (1,43)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HD11 | 8        | 0.24          |
| (1,43)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HD12 | 14       | 0.24          |
| (1,43)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HD12 | 16       | 0.24          |
| (1,43)  | 1:31:A:LEU:HD22 | 1:31:A:LEU:HD13 | 20       | 0.24          |
| (2,62)  | 1:27:A:4PH:HD1  | 1:4:A:LYS:HG3   | 18       | 0.23          |
| (2,50)  | 1:27:A:4PH:HD2  | 1:31:A:LEU:HD22 | 12       | 0.23          |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33B | 1        | 0.23          |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33  | 2        | 0.23          |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33A | 3        | 0.23          |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33B | 9        | 0.23          |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33B | 14       | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33A | 16       | 0.23          |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33B | 19       | 0.23          |
| (2,20)  | 1:18:A:ALA:HB3  | 1:15:A:GLU:HA   | 3        | 0.23          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 1        | 0.23          |
| (1,296) | 1:31:A:LEU:HD22 | 1:27:A:4PH:H33A | 10       | 0.23          |
| (1,296) | 1:31:A:LEU:HD22 | 1:27:A:4PH:H33A | 14       | 0.23          |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 14       | 0.23          |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 18       | 0.23          |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 20       | 0.23          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 15       | 0.23          |
| (1,112) | 1:20:A:4PH:HD2  | 1:17:A:LEU:HD23 | 17       | 0.23          |
| (1,52)  | 1:0:A:ACE:H2    | 1:1:A:PRO:HD2   | 14       | 0.23          |
| (2,85)  | 1:8:A:PRO:HD2   | 1:20:A:4PH:HD2  | 13       | 0.22          |
| (2,71)  | 1:20:A:4PH:H    | 1:20:A:4PH:HD1  | 16       | 0.22          |
| (2,39)  | 1:20:A:4PH:HE1  | 1:20:A:4PH:H33B | 11       | 0.22          |
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 15       | 0.22          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 2        | 0.22          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 13       | 0.22          |
| (1,112) | 1:20:A:4PH:HD2  | 1:17:A:LEU:HD21 | 15       | 0.22          |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG21  | 7        | 0.22          |
| (1,107) | 1:13:A:THR:H    | 1:12:A:ALA:HB3  | 14       | 0.22          |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 10       | 0.22          |
| (1,373) | 1:27:A:4PH:HD2  | 1:4:A:LYS:HA    | 10       | 0.21          |
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 12       | 0.21          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 5        | 0.21          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 8        | 0.21          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 17       | 0.21          |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 2        | 0.21          |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 4        | 0.21          |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 5        | 0.21          |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 7        | 0.21          |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 8        | 0.21          |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 10       | 0.21          |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 11       | 0.21          |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 12       | 0.21          |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 13       | 0.21          |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 14       | 0.21          |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 15       | 0.21          |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 16       | 0.21          |
| (1,124) | 1:11:A:ASN:HB3  | 1:11:A:ASN:HD22 | 20       | 0.21          |
| (1,91)  | 1:27:A:4PH:HE1  | 1:2:A:PRO:HB3   | 2        | 0.21          |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 9        | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 7        | 0.2           |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 11       | 0.2           |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 18       | 0.2           |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 1        | 0.2           |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 3        | 0.2           |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 6        | 0.2           |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 9        | 0.2           |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 17       | 0.2           |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 19       | 0.2           |
| (1,93)  | 1:34:A:4PH:HD1  | 1:0:A:ACE:H2    | 9        | 0.2           |
| (1,93)  | 1:34:A:4PH:HD2  | 1:0:A:ACE:H1    | 11       | 0.2           |
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 6        | 0.19          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 3        | 0.19          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 10       | 0.19          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 12       | 0.19          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 14       | 0.19          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 15       | 0.19          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 19       | 0.19          |
| (1,296) | 1:31:A:LEU:HD21 | 1:27:A:4PH:H33  | 5        | 0.19          |
| (1,295) | 1:4:A:LYS:HG2   | 1:4:A:LYS:HB2   | 20       | 0.19          |
| (1,266) | 1:26:A:LYS:HG2  | 1:26:A:LYS:H    | 9        | 0.19          |
| (1,266) | 1:26:A:LYS:HG2  | 1:26:A:LYS:H    | 19       | 0.19          |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 6        | 0.19          |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 18       | 0.19          |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 2        | 0.19          |
| (1,80)  | 1:27:A:4PH:HD1  | 1:24:A:LEU:HA   | 15       | 0.19          |
| (1,74)  | 1:3:A:THR:HA    | 1:27:A:4PH:HE1  | 3        | 0.19          |
| (1,43)  | 1:31:A:LEU:HD21 | 1:31:A:LEU:HD11 | 18       | 0.19          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 4        | 0.18          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 16       | 0.18          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 20       | 0.18          |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 4        | 0.18          |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 19       | 0.18          |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 19       | 0.18          |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG21  | 6        | 0.18          |
| (1,91)  | 1:27:A:4PH:HE1  | 1:2:A:PRO:HB3   | 14       | 0.18          |
| (1,43)  | 1:31:A:LEU:HD23 | 1:31:A:LEU:HD13 | 12       | 0.18          |
| (1,21)  | 1:34:A:4PH:HA   | 1:0:A:ACE:H3    | 12       | 0.18          |
| (1,19)  | 1:30:A:ASP:HA   | 1:33:A:ASP:HB3  | 18       | 0.18          |
| (2,110) | 1:27:A:4PH:HD2  | 1:5:A:PRO:HG2   | 6        | 0.17          |
| (2,13)  | 1:24:A:LEU:HD11 | 1:5:A:PRO:HG2   | 20       | 0.17          |
| (1,378) | 1:4:A:LYS:HG3   | 1:27:A:4PH:HE1  | 9        | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 17       | 0.17          |
| (1,343) | 1:4:A:LYS:HB2   | 1:4:A:LYS:H     | 9        | 0.17          |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 5        | 0.17          |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 11       | 0.17          |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 17       | 0.17          |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 8        | 0.17          |
| (1,112) | 1:20:A:4PH:HD2  | 1:17:A:LEU:HD22 | 5        | 0.17          |
| (1,112) | 1:20:A:4PH:HD1  | 1:17:A:LEU:HD23 | 11       | 0.17          |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 3        | 0.17          |
| (2,110) | 1:27:A:4PH:HD2  | 1:5:A:PRO:HG2   | 15       | 0.16          |
| (2,36)  | 1:8:A:PRO:HD3   | 1:20:A:4PH:HD2  | 11       | 0.16          |
| (1,296) | 1:31:A:LEU:HD23 | 1:27:A:4PH:H33A | 7        | 0.16          |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 1        | 0.16          |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 3        | 0.16          |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 8        | 0.16          |
| (1,138) | 1:28:A:GLN:HA   | 1:27:A:4PH:HD1  | 3        | 0.16          |
| (1,112) | 1:20:A:4PH:HD1  | 1:17:A:LEU:HD23 | 16       | 0.16          |
| (1,12)  | 1:17:A:LEU:HA   | 1:17:A:LEU:HD22 | 20       | 0.16          |
| (2,41)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HB3   | 2        | 0.15          |
| (2,13)  | 1:24:A:LEU:HD13 | 1:5:A:PRO:HG2   | 3        | 0.15          |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 2        | 0.15          |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 3        | 0.15          |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 8        | 0.15          |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 13       | 0.15          |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 15       | 0.15          |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 17       | 0.15          |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 14       | 0.15          |
| (1,93)  | 1:34:A:4PH:HD1  | 1:0:A:ACE:H2    | 3        | 0.15          |
| (1,25)  | 1:18:A:ALA:HA   | 1:18:A:ALA:HB3  | 1        | 0.15          |
| (1,25)  | 1:18:A:ALA:HA   | 1:18:A:ALA:HB2  | 2        | 0.15          |
| (1,25)  | 1:18:A:ALA:HA   | 1:18:A:ALA:HB1  | 3        | 0.15          |
| (1,25)  | 1:18:A:ALA:HA   | 1:18:A:ALA:HB2  | 4        | 0.15          |
| (1,25)  | 1:18:A:ALA:HA   | 1:18:A:ALA:HB3  | 6        | 0.15          |
| (1,25)  | 1:18:A:ALA:HA   | 1:18:A:ALA:HB2  | 14       | 0.15          |
| (1,25)  | 1:18:A:ALA:HA   | 1:18:A:ALA:HB2  | 17       | 0.15          |
| (2,85)  | 1:8:A:PRO:HD2   | 1:20:A:4PH:HD2  | 8        | 0.14          |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 4        | 0.14          |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 6        | 0.14          |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 9        | 0.14          |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 10       | 0.14          |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 14       | 0.14          |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 18       | 0.14          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,327) | 1:28:A:GLN:HB3 | 1:28:A:GLN:H    | 20       | 0.14          |
| (1,246) | 1:3:A:THR:H    | 1:3:A:THR:HB    | 2        | 0.14          |
| (1,246) | 1:3:A:THR:H    | 1:3:A:THR:HB    | 10       | 0.14          |
| (1,246) | 1:3:A:THR:H    | 1:3:A:THR:HB    | 16       | 0.14          |
| (1,138) | 1:28:A:GLN:HA  | 1:27:A:4PH:HD1  | 6        | 0.14          |
| (1,112) | 1:20:A:4PH:HD2 | 1:17:A:LEU:HD21 | 8        | 0.14          |
| (1,49)  | 1:8:A:PRO:HB3  | 1:12:A:ALA:HB2  | 10       | 0.14          |
| (1,34)  | 1:5:A:PRO:HD2  | 1:24:A:LEU:HD11 | 7        | 0.14          |
| (1,25)  | 1:18:A:ALA:HA  | 1:18:A:ALA:HB3  | 5        | 0.14          |
| (1,25)  | 1:18:A:ALA:HA  | 1:18:A:ALA:HB1  | 7        | 0.14          |
| (1,25)  | 1:18:A:ALA:HA  | 1:18:A:ALA:HB1  | 10       | 0.14          |
| (1,25)  | 1:18:A:ALA:HA  | 1:18:A:ALA:HB1  | 11       | 0.14          |
| (1,25)  | 1:18:A:ALA:HA  | 1:18:A:ALA:HB3  | 13       | 0.14          |
| (1,25)  | 1:18:A:ALA:HA  | 1:18:A:ALA:HB2  | 16       | 0.14          |
| (1,25)  | 1:18:A:ALA:HA  | 1:18:A:ALA:HB1  | 18       | 0.14          |
| (1,25)  | 1:18:A:ALA:HA  | 1:18:A:ALA:HB3  | 19       | 0.14          |
| (1,24)  | 1:22:A:ALA:HB2 | 1:22:A:ALA:HA   | 2        | 0.14          |
| (2,67)  | 1:7:A:LYS:H    | 1:7:A:LYS:HD2   | 5        | 0.13          |
| (2,48)  | 1:25:A:ALA:H   | 1:24:A:LEU:HD21 | 11       | 0.13          |
| (2,36)  | 1:8:A:PRO:HD3  | 1:20:A:4PH:HD1  | 3        | 0.13          |
| (1,364) | 1:0:A:ACE:H2   | 1:34:A:4PH:HB3  | 9        | 0.13          |
| (1,358) | 1:18:A:ALA:H   | 1:17:A:LEU:HB2  | 7        | 0.13          |
| (1,352) | 1:27:A:4PH:HE1 | 1:2:A:PRO:HG3   | 9        | 0.13          |
| (1,327) | 1:28:A:GLN:HB3 | 1:28:A:GLN:H    | 1        | 0.13          |
| (1,327) | 1:28:A:GLN:HB3 | 1:28:A:GLN:H    | 5        | 0.13          |
| (1,327) | 1:28:A:GLN:HB3 | 1:28:A:GLN:H    | 7        | 0.13          |
| (1,327) | 1:28:A:GLN:HB3 | 1:28:A:GLN:H    | 12       | 0.13          |
| (1,327) | 1:28:A:GLN:HB3 | 1:28:A:GLN:H    | 16       | 0.13          |
| (1,327) | 1:28:A:GLN:HB3 | 1:28:A:GLN:H    | 19       | 0.13          |
| (1,240) | 1:20:A:4PH:HD1 | 1:21:A:GLN:HE21 | 16       | 0.13          |
| (1,240) | 1:20:A:4PH:HD1 | 1:21:A:GLN:HE21 | 20       | 0.13          |
| (1,209) | 1:20:A:4PH:HE1 | 1:7:A:LYS:HA    | 6        | 0.13          |
| (1,109) | 1:7:A:LYS:H    | 1:6:A:THR:HG23  | 15       | 0.13          |
| (1,93)  | 1:34:A:4PH:HD2 | 1:0:A:ACE:H3    | 5        | 0.13          |
| (1,93)  | 1:34:A:4PH:HD2 | 1:0:A:ACE:H2    | 17       | 0.13          |
| (1,34)  | 1:5:A:PRO:HD2  | 1:24:A:LEU:HD11 | 5        | 0.13          |
| (1,25)  | 1:18:A:ALA:HA  | 1:18:A:ALA:HB3  | 8        | 0.13          |
| (1,25)  | 1:18:A:ALA:HA  | 1:18:A:ALA:HB3  | 12       | 0.13          |
| (1,25)  | 1:18:A:ALA:HA  | 1:18:A:ALA:HB1  | 15       | 0.13          |
| (1,24)  | 1:22:A:ALA:HB3 | 1:22:A:ALA:HA   | 1        | 0.13          |
| (1,24)  | 1:22:A:ALA:HB1 | 1:22:A:ALA:HA   | 4        | 0.13          |
| (1,24)  | 1:22:A:ALA:HB3 | 1:22:A:ALA:HA   | 5        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,24)  | 1:22:A:ALA:HB1  | 1:22:A:ALA:HA   | 6        | 0.13          |
| (1,24)  | 1:22:A:ALA:HB3  | 1:22:A:ALA:HA   | 7        | 0.13          |
| (1,24)  | 1:22:A:ALA:HB3  | 1:22:A:ALA:HA   | 10       | 0.13          |
| (1,24)  | 1:22:A:ALA:HB2  | 1:22:A:ALA:HA   | 11       | 0.13          |
| (1,24)  | 1:22:A:ALA:HB2  | 1:22:A:ALA:HA   | 12       | 0.13          |
| (1,24)  | 1:22:A:ALA:HB2  | 1:22:A:ALA:HA   | 13       | 0.13          |
| (1,24)  | 1:22:A:ALA:HB1  | 1:22:A:ALA:HA   | 14       | 0.13          |
| (1,24)  | 1:22:A:ALA:HB3  | 1:22:A:ALA:HA   | 16       | 0.13          |
| (1,24)  | 1:22:A:ALA:HB2  | 1:22:A:ALA:HA   | 17       | 0.13          |
| (1,24)  | 1:22:A:ALA:HB3  | 1:22:A:ALA:HA   | 19       | 0.13          |
| (2,67)  | 1:7:A:LYS:H     | 1:7:A:LYS:HD2   | 7        | 0.12          |
| (2,49)  | 1:20:A:4PH:HD2  | 1:24:A:LEU:HD23 | 3        | 0.12          |
| (2,48)  | 1:25:A:ALA:H    | 1:24:A:LEU:HD22 | 16       | 0.12          |
| (2,36)  | 1:8:A:PRO:HD3   | 1:20:A:4PH:HD1  | 6        | 0.12          |
| (2,36)  | 1:8:A:PRO:HD3   | 1:20:A:4PH:HD2  | 19       | 0.12          |
| (1,327) | 1:28:A:GLN:HB3  | 1:28:A:GLN:H    | 11       | 0.12          |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 9        | 0.12          |
| (1,209) | 1:20:A:4PH:HE1  | 1:7:A:LYS:HA    | 14       | 0.12          |
| (1,116) | 1:20:A:4PH:HE2  | 1:24:A:LEU:HD23 | 19       | 0.12          |
| (1,109) | 1:7:A:LYS:H     | 1:6:A:THR:HG21  | 20       | 0.12          |
| (1,104) | 1:13:A:THR:H    | 1:13:A:THR:HG21 | 5        | 0.12          |
| (1,40)  | 1:4:A:LYS:HG2   | 1:27:A:4PH:H33  | 17       | 0.12          |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 5        | 0.12          |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 14       | 0.12          |
| (1,35)  | 1:5:A:PRO:HD2   | 1:4:A:LYS:HG3   | 16       | 0.12          |
| (1,34)  | 1:5:A:PRO:HD2   | 1:24:A:LEU:HD11 | 2        | 0.12          |
| (1,25)  | 1:18:A:ALA:HA   | 1:18:A:ALA:HB1  | 9        | 0.12          |
| (1,25)  | 1:18:A:ALA:HA   | 1:18:A:ALA:HB3  | 20       | 0.12          |
| (1,24)  | 1:22:A:ALA:HB3  | 1:22:A:ALA:HA   | 3        | 0.12          |
| (1,24)  | 1:22:A:ALA:HB3  | 1:22:A:ALA:HA   | 8        | 0.12          |
| (1,24)  | 1:22:A:ALA:HB3  | 1:22:A:ALA:HA   | 9        | 0.12          |
| (1,24)  | 1:22:A:ALA:HB1  | 1:22:A:ALA:HA   | 15       | 0.12          |
| (1,24)  | 1:22:A:ALA:HB3  | 1:22:A:ALA:HA   | 18       | 0.12          |
| (1,24)  | 1:22:A:ALA:HB1  | 1:22:A:ALA:HA   | 20       | 0.12          |
| (1,12)  | 1:17:A:LEU:HA   | 1:17:A:LEU:HD23 | 12       | 0.12          |
| (2,41)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HB3   | 4        | 0.11          |
| (2,27)  | 1:34:A:4PH:HE1  | 1:1:A:PRO:HA    | 10       | 0.11          |
| (1,373) | 1:27:A:4PH:HD2  | 1:4:A:LYS:HA    | 2        | 0.11          |
| (1,352) | 1:27:A:4PH:HE1  | 1:2:A:PRO:HG3   | 16       | 0.11          |
| (1,296) | 1:31:A:LEU:HD22 | 1:27:A:4PH:H33  | 2        | 0.11          |
| (1,296) | 1:31:A:LEU:HD23 | 1:27:A:4PH:H33  | 3        | 0.11          |
| (1,246) | 1:3:A:THR:H     | 1:3:A:THR:HB    | 7        | 0.11          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,246) | 1:3:A:THR:H    | 1:3:A:THR:HB    | 13       | 0.11          |
| (1,246) | 1:3:A:THR:H    | 1:3:A:THR:HB    | 20       | 0.11          |
| (1,240) | 1:20:A:4PH:HD2 | 1:21:A:GLN:HE21 | 13       | 0.11          |
| (1,198) | 1:27:A:4PH:HD2 | 1:27:A:4PH:HB3  | 15       | 0.11          |
| (1,109) | 1:7:A:LYS:H    | 1:6:A:THR:HG22  | 18       | 0.11          |
| (1,104) | 1:13:A:THR:H   | 1:13:A:THR:HG22 | 9        | 0.11          |
| (1,74)  | 1:3:A:THR:HA   | 1:27:A:4PH:HE1  | 20       | 0.11          |
| (1,12)  | 1:17:A:LEU:HA  | 1:17:A:LEU:HD23 | 8        | 0.11          |
| (2,36)  | 1:8:A:PRO:HD3  | 1:20:A:4PH:HD1  | 8        | 0.1           |
| (1,246) | 1:3:A:THR:H    | 1:3:A:THR:HB    | 12       | 0.1           |
| (1,112) | 1:20:A:4PH:HD1 | 1:17:A:LEU:HD23 | 19       | 0.1           |
| (1,21)  | 1:34:A:4PH:HA  | 1:0:A:ACE:H1    | 1        | 0.1           |
| (1,12)  | 1:17:A:LEU:HA  | 1:17:A:LEU:HD22 | 1        | 0.1           |



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

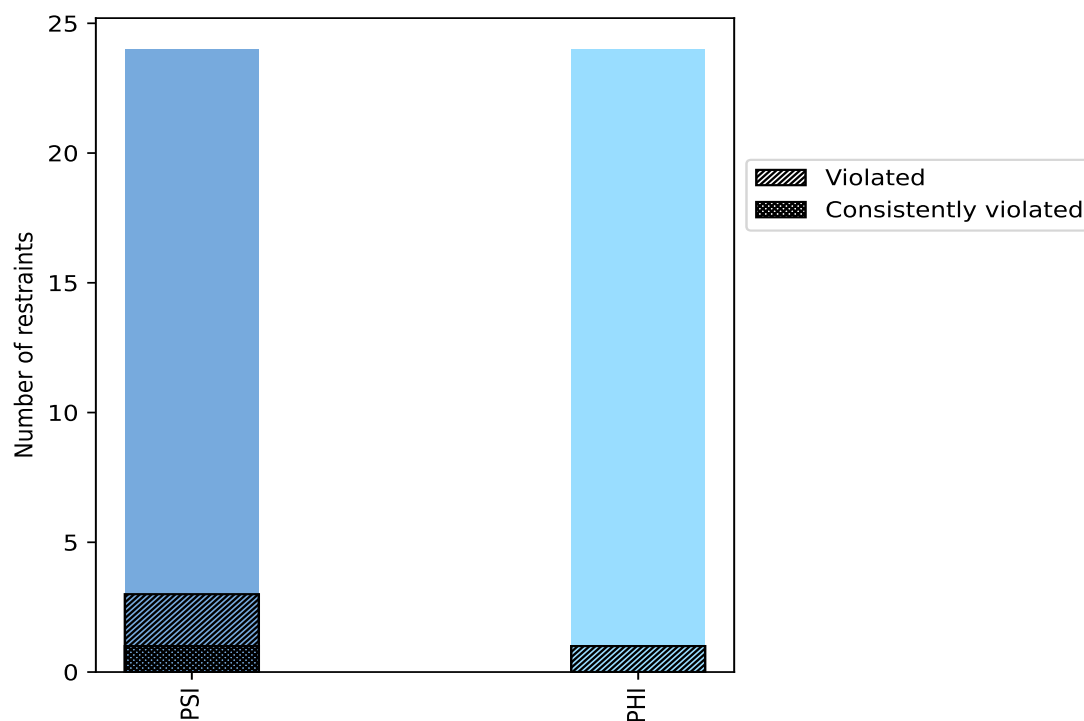
### 10.1 Summary of dihedral-angle violations [i](#)

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        | 24    | 50.0           | 3                     | 12.5           | 6.2            | 1                                  | 4.2            | 2.1            |
| PHI        | 24    | 50.0           | 1                     | 4.2            | 2.1            | 0                                  | 0.0            | 0.0            |
| Total      | 48    | 100.0          | 4                     | 8.3            | 8.3            | 1                                  | 2.1            | 2.1            |

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

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



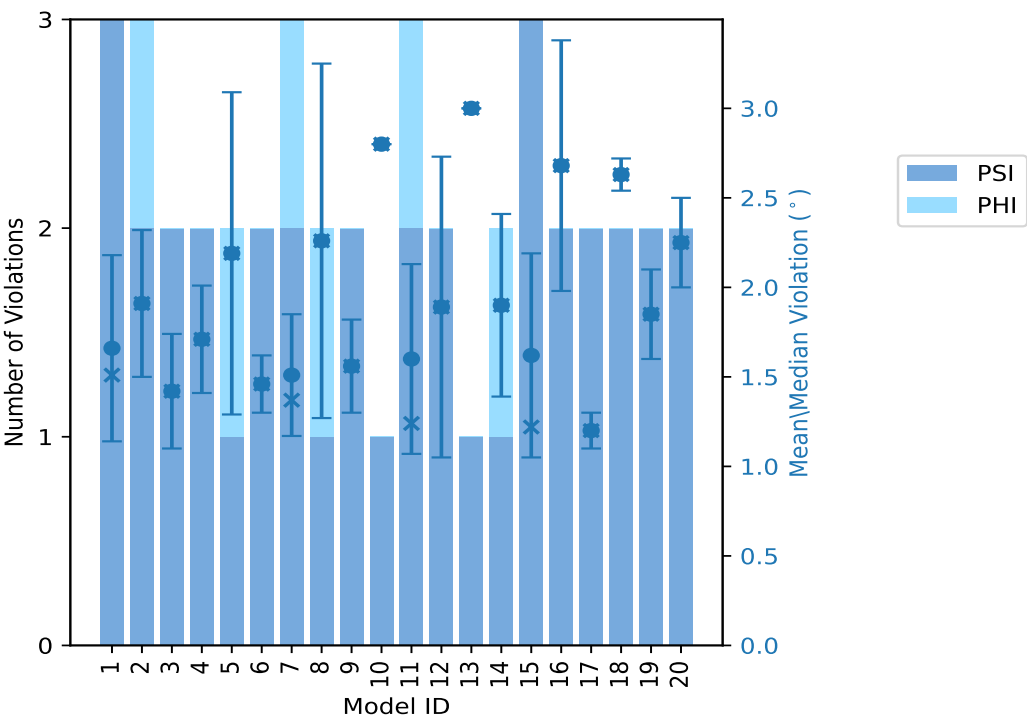
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model ⓘ

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 3                    | 0   | 3     | 1.66     | 2.36    | 0.52   | 1.51       |
| 2        | 2                    | 1   | 3     | 1.91     | 2.41    | 0.41   | 1.91       |
| 3        | 2                    | 0   | 2     | 1.42     | 1.74    | 0.32   | 1.42       |
| 4        | 2                    | 0   | 2     | 1.71     | 2.01    | 0.3    | 1.71       |
| 5        | 1                    | 1   | 2     | 2.19     | 3.09    | 0.9    | 2.19       |
| 6        | 2                    | 0   | 2     | 1.46     | 1.62    | 0.16   | 1.46       |
| 7        | 2                    | 1   | 3     | 1.51     | 1.98    | 0.34   | 1.37       |
| 8        | 1                    | 1   | 2     | 2.26     | 3.24    | 0.99   | 2.26       |
| 9        | 2                    | 0   | 2     | 1.56     | 1.82    | 0.26   | 1.56       |
| 10       | 1                    | 0   | 1     | 2.8      | 2.8     | 0.0    | 2.8        |
| 11       | 2                    | 1   | 3     | 1.6      | 2.35    | 0.53   | 1.24       |
| 12       | 2                    | 0   | 2     | 1.89     | 2.73    | 0.84   | 1.89       |
| 13       | 1                    | 0   | 1     | 3.0      | 3.0     | 0.0    | 3.0        |
| 14       | 1                    | 1   | 2     | 1.9      | 2.41    | 0.51   | 1.9        |
| 15       | 3                    | 0   | 3     | 1.62     | 2.43    | 0.57   | 1.22       |
| 16       | 2                    | 0   | 2     | 2.68     | 3.38    | 0.7    | 2.68       |
| 17       | 2                    | 0   | 2     | 1.2      | 1.31    | 0.1    | 1.2        |
| 18       | 2                    | 0   | 2     | 2.63     | 2.72    | 0.09   | 2.63       |
| 19       | 2                    | 0   | 2     | 1.85     | 2.1     | 0.25   | 1.85       |
| 20       | 2                    | 0   | 2     | 2.25     | 2.5     | 0.25   | 2.25       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

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

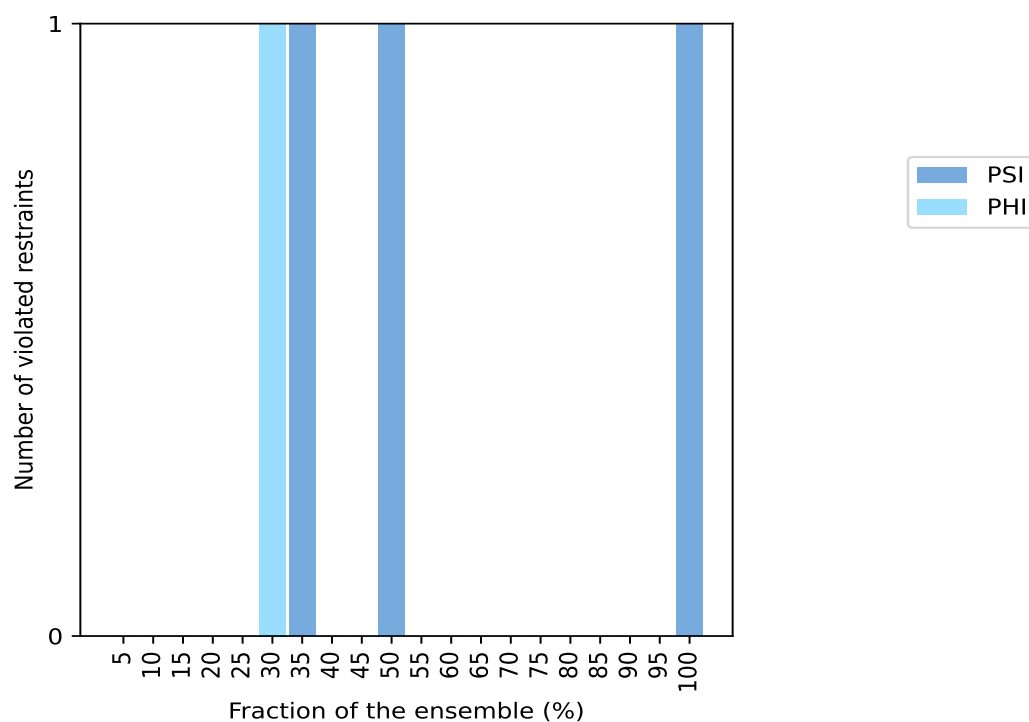
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |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

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

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

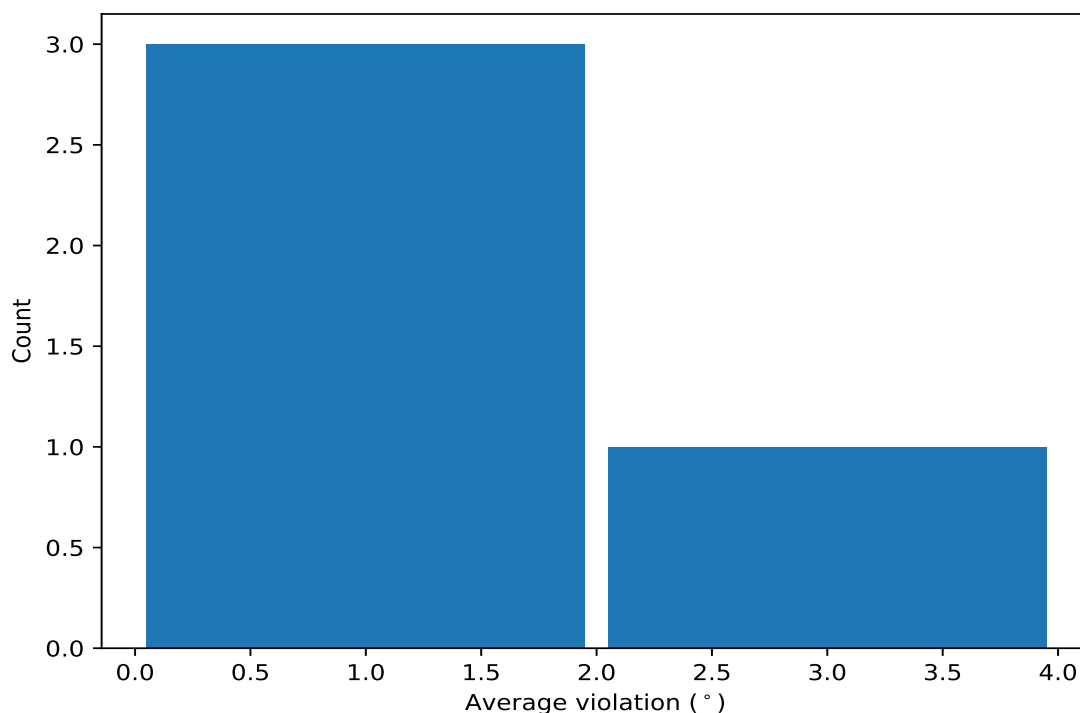


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

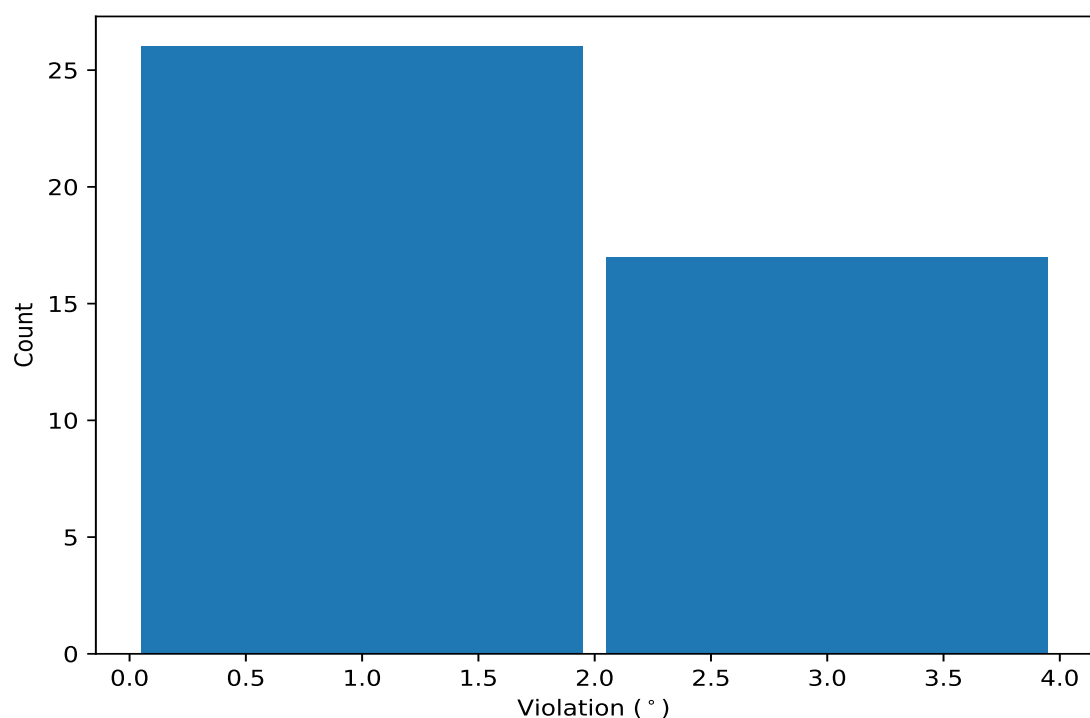
| Key    | Atom-1       | Atom-2        | Atom-3       | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|--------------|---------------|--------------|--------------|---------------------|------|-----------------|--------|
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 20                  | 2.39 | 0.54            | 2.41   |
| (1,8)  | 1:9:A:GLY:N  | 1:9:A:GLY:CA  | 1:9:A:GLY:C  | 1:10:A:ASP:N | 10                  | 1.34 | 0.26            | 1.31   |
| (1,12) | 1:12:A:ALA:N | 1:12:A:ALA:CA | 1:12:A:ALA:C | 1:13:A:THR:N | 7                   | 1.68 | 0.53            | 1.6    |
| (1,7)  | 1:8:A:PRO:C  | 1:9:A:GLY:N   | 1:9:A:GLY:CA | 1:9:A:GLY:C  | 6                   | 1.29 | 0.08            | 1.28   |

<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 (°) |
|--------|--------------|---------------|--------------|--------------|----------|---------------|
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 16       | 3.38          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 8        | 3.24          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 5        | 3.09          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 13       | 3.0           |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 10       | 2.8           |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 12       | 2.73          |
| (1,12) | 1:12:A:ALA:N | 1:12:A:ALA:CA | 1:12:A:ALA:C | 1:13:A:THR:N | 18       | 2.72          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 18       | 2.54          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 20       | 2.5           |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 15       | 2.43          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 2        | 2.41          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 14       | 2.41          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 1        | 2.36          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 11       | 2.35          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 19       | 2.1           |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 4        | 2.01          |
| (1,8)  | 1:9:A:GLY:N  | 1:9:A:GLY:CA  | 1:9:A:GLY:C  | 1:10:A:ASP:N | 20       | 2.0           |
| (1,12) | 1:12:A:ALA:N | 1:12:A:ALA:CA | 1:12:A:ALA:C | 1:13:A:THR:N | 16       | 1.98          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 7        | 1.98          |
| (1,12) | 1:12:A:ALA:N | 1:12:A:ALA:CA | 1:12:A:ALA:C | 1:13:A:THR:N | 2        | 1.91          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 9        | 1.82          |

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| Key    | Atom-1       | Atom-2        | Atom-3       | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|--------------|--------------|----------|---------------|
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 3        | 1.74          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 6        | 1.62          |
| (1,12) | 1:12:A:ALA:N | 1:12:A:ALA:CA | 1:12:A:ALA:C | 1:13:A:THR:N | 19       | 1.6           |
| (1,8)  | 1:9:A:GLY:N  | 1:9:A:GLY:CA  | 1:9:A:GLY:C  | 1:10:A:ASP:N | 1        | 1.51          |
| (1,8)  | 1:9:A:GLY:N  | 1:9:A:GLY:CA  | 1:9:A:GLY:C  | 1:10:A:ASP:N | 4        | 1.41          |
| (1,7)  | 1:8:A:PRO:C  | 1:9:A:GLY:N   | 1:9:A:GLY:CA | 1:9:A:GLY:C  | 2        | 1.4           |
| (1,7)  | 1:8:A:PRO:C  | 1:9:A:GLY:N   | 1:9:A:GLY:CA | 1:9:A:GLY:C  | 14       | 1.39          |
| (1,8)  | 1:9:A:GLY:N  | 1:9:A:GLY:CA  | 1:9:A:GLY:C  | 1:10:A:ASP:N | 7        | 1.37          |
| (1,10) | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 1:12:A:ALA:N | 17       | 1.31          |
| (1,8)  | 1:9:A:GLY:N  | 1:9:A:GLY:CA  | 1:9:A:GLY:C  | 1:10:A:ASP:N | 9        | 1.31          |
| (1,8)  | 1:9:A:GLY:N  | 1:9:A:GLY:CA  | 1:9:A:GLY:C  | 1:10:A:ASP:N | 6        | 1.3           |
| (1,7)  | 1:8:A:PRO:C  | 1:9:A:GLY:N   | 1:9:A:GLY:CA | 1:9:A:GLY:C  | 5        | 1.29          |
| (1,7)  | 1:8:A:PRO:C  | 1:9:A:GLY:N   | 1:9:A:GLY:CA | 1:9:A:GLY:C  | 8        | 1.27          |
| (1,12) | 1:12:A:ALA:N | 1:12:A:ALA:CA | 1:12:A:ALA:C | 1:13:A:THR:N | 11       | 1.24          |
| (1,8)  | 1:9:A:GLY:N  | 1:9:A:GLY:CA  | 1:9:A:GLY:C  | 1:10:A:ASP:N | 15       | 1.22          |
| (1,12) | 1:12:A:ALA:N | 1:12:A:ALA:CA | 1:12:A:ALA:C | 1:13:A:THR:N | 15       | 1.21          |
| (1,7)  | 1:8:A:PRO:C  | 1:9:A:GLY:N   | 1:9:A:GLY:CA | 1:9:A:GLY:C  | 11       | 1.2           |
| (1,7)  | 1:8:A:PRO:C  | 1:9:A:GLY:N   | 1:9:A:GLY:CA | 1:9:A:GLY:C  | 7        | 1.19          |
| (1,12) | 1:12:A:ALA:N | 1:12:A:ALA:CA | 1:12:A:ALA:C | 1:13:A:THR:N | 1        | 1.12          |
| (1,8)  | 1:9:A:GLY:N  | 1:9:A:GLY:CA  | 1:9:A:GLY:C  | 1:10:A:ASP:N | 3        | 1.1           |
| (1,8)  | 1:9:A:GLY:N  | 1:9:A:GLY:CA  | 1:9:A:GLY:C  | 1:10:A:ASP:N | 17       | 1.1           |
| (1,8)  | 1:9:A:GLY:N  | 1:9:A:GLY:CA  | 1:9:A:GLY:C  | 1:10:A:ASP:N | 12       | 1.05          |