



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 01:44 PM UTC

PDB ID : 5NMY / pdb\_00005nmy  
BMRB ID : 34121  
Title : NMR solution structure of lysostaphin  
Authors : Tossavainen, H.; Raulinaitis, V.; Permi, P.  
Deposited on : 2017-04-07

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

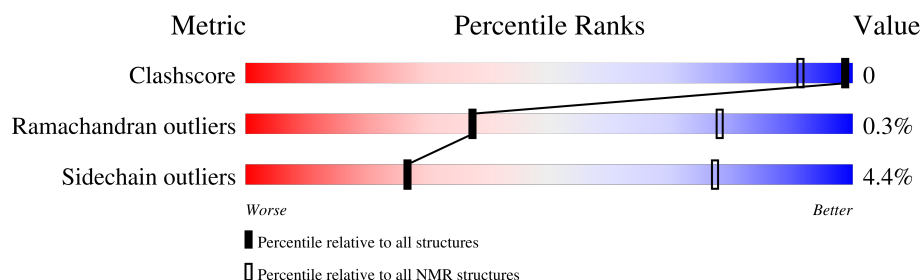
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 85%.

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     | 245    |                  |

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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

| Well-defined (core) protein residues |                                                                |                   |              |
|--------------------------------------|----------------------------------------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)                                          | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:253-A:268, A:278-A:304,<br>A:313-A:350, A:360-A:388<br>(110) | 0.53              | 10           |
| 2                                    | A:402-A:465, A:470-A:493<br>(88)                               | 0.44              | 6            |

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

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

The models can be grouped into 5 clusters. No single-model clusters were found.

| Cluster number | Models       |
|----------------|--------------|
| 1              | 2, 3, 7, 14  |
| 2              | 8, 9, 10, 15 |
| 3              | 1, 11, 12    |
| 4              | 5, 13        |
| 5              | 4, 6         |

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3722 atoms, of which 1823 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lysostaphin.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|-------|
| 1   | A     | 245      | Total | C    | H    | N   | O   | S | 0     |
|     |       |          | 3721  | 1208 | 1823 | 331 | 352 | 7 |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 249     | GLY      | -      | expression tag | UNP P10547 |
| A     | 250     | SER      | -      | expression tag | UNP P10547 |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

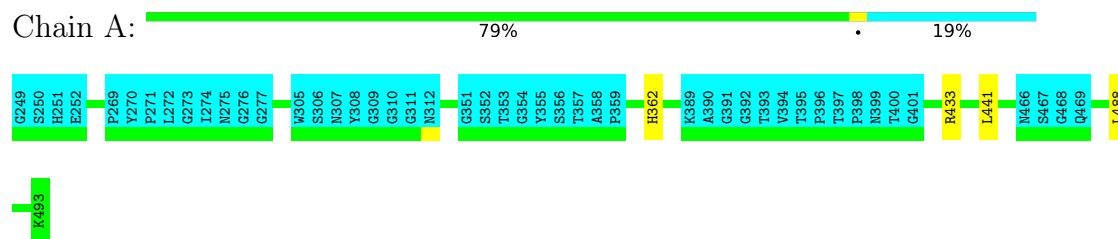
| Mol | Chain | Residues | Atoms |    |
|-----|-------|----------|-------|----|
| 2   | A     | 1        | Total | Zn |
|     |       |          | 1     | 1  |

## 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: Lysostaphin

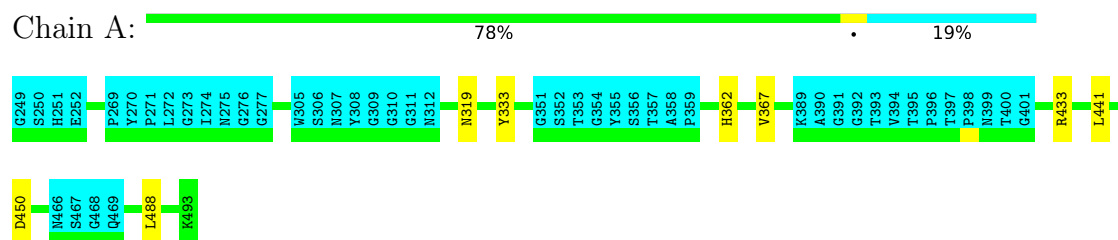


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

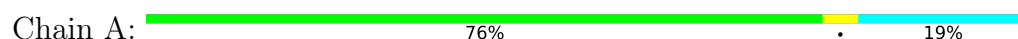
#### 4.2.1 Score per residue for model 1

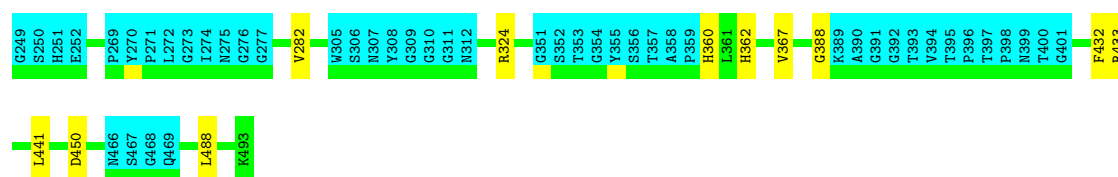
- Molecule 1: Lysostaphin



#### 4.2.2 Score per residue for model 2

- Molecule 1: Lysostaphin

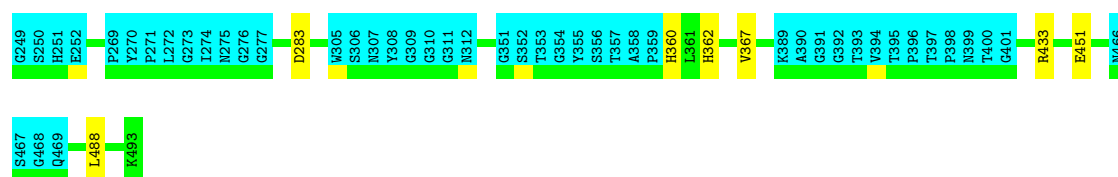




### 4.2.3 Score per residue for model 3

- Molecule 1: Lysostaphin

Chain A: 78% 19%



### 4.2.4 Score per residue for model 4

- Molecule 1: Lysostaphin

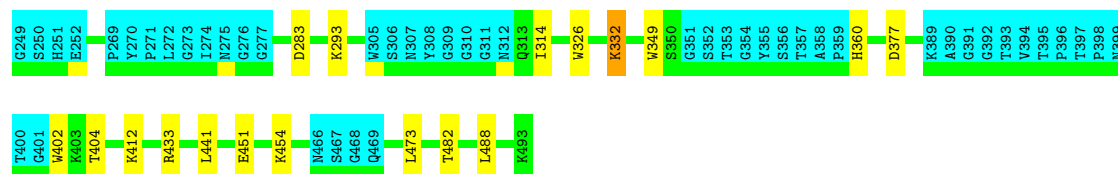
Chain A: 76% 5% 19%



### 4.2.5 Score per residue for model 5

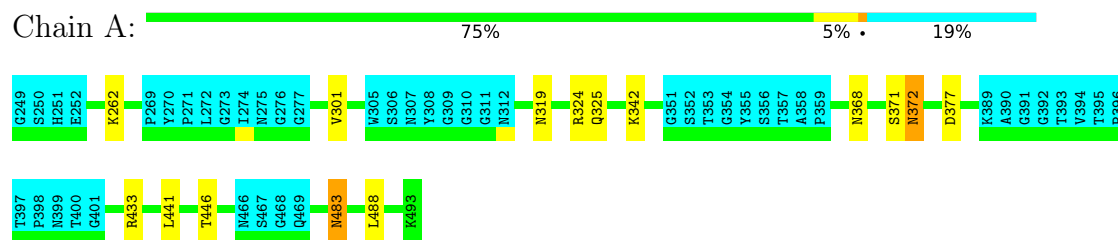
- Molecule 1: Lysostaphin

Chain A: 73% 7% 19%



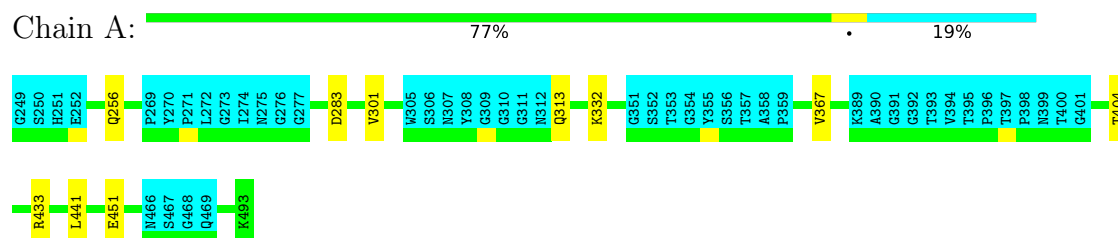
### 4.2.6 Score per residue for model 6

- Molecule 1: Lysostaphin



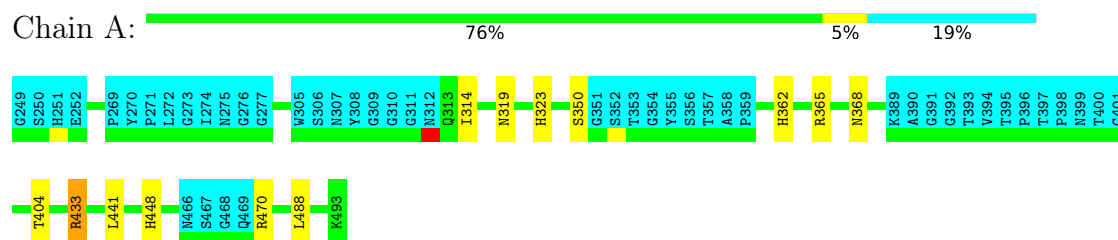
#### 4.2.7 Score per residue for model 7

- Molecule 1: Lysostaphin



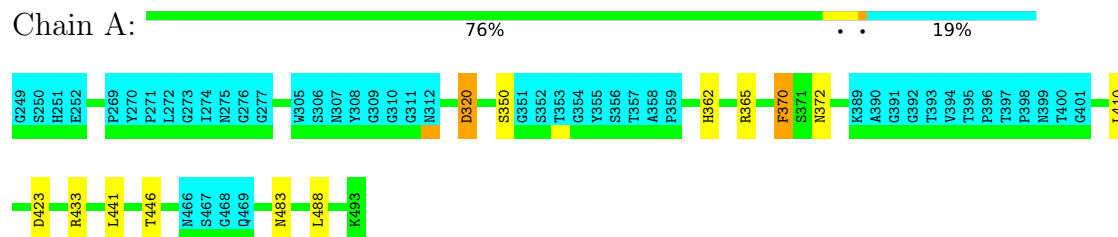
#### 4.2.8 Score per residue for model 8

- Molecule 1: Lysostaphin



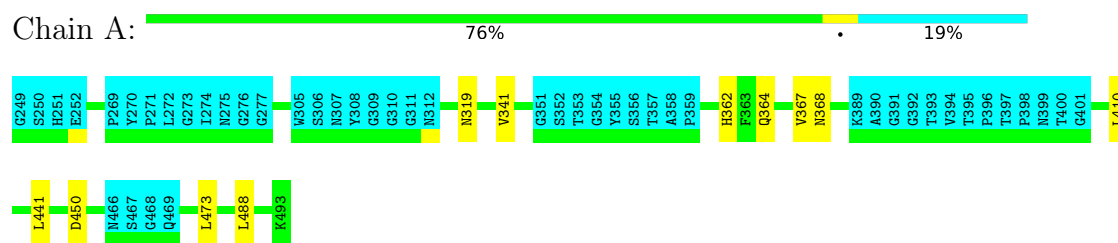
#### 4.2.9 Score per residue for model 9

- Molecule 1: Lysostaphin



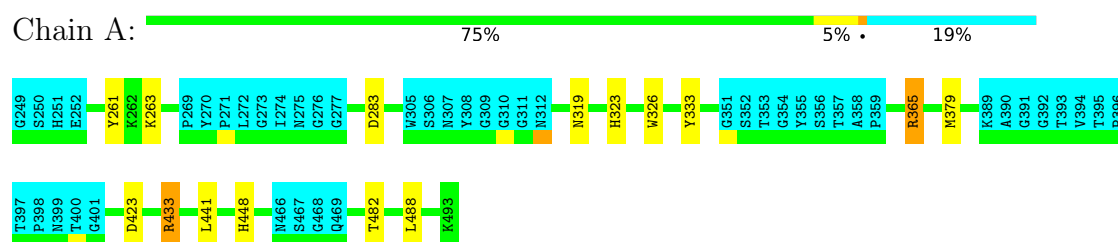
#### 4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Lysostaphin



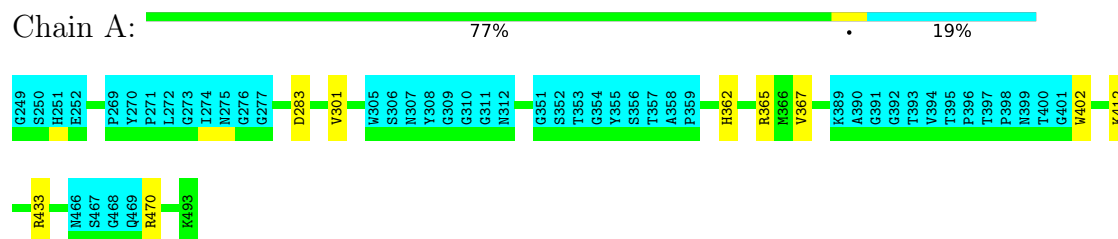
#### 4.2.11 Score per residue for model 11

- Molecule 1: Lysostaphin



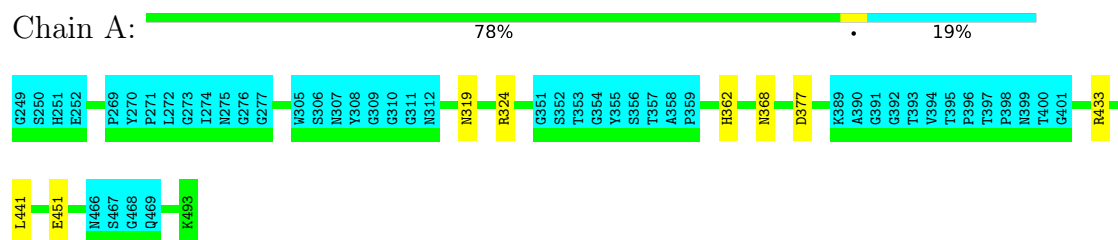
#### 4.2.12 Score per residue for model 12

- Molecule 1: Lysostaphin



#### 4.2.13 Score per residue for model 13

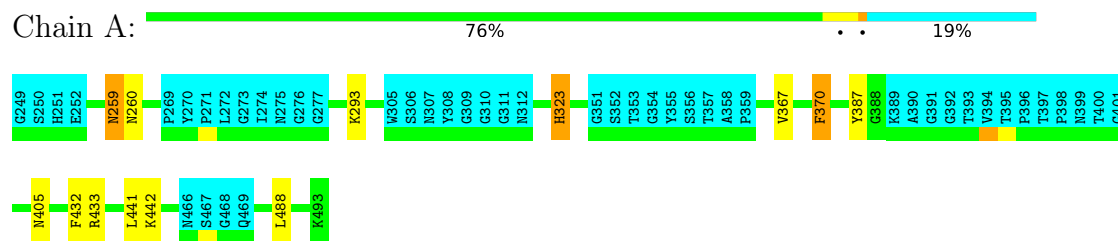
- Molecule 1: Lysostaphin





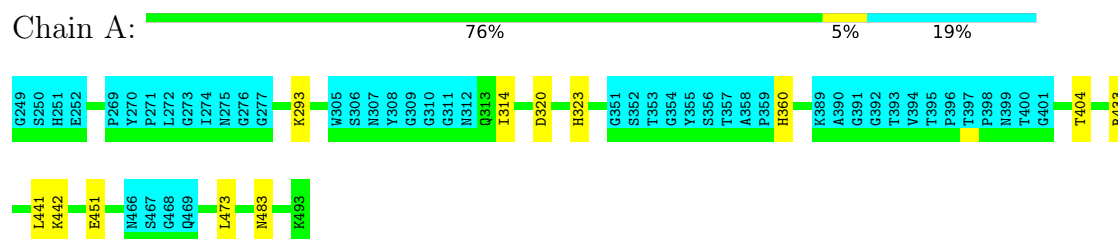
#### 4.2.14 Score per residue for model 14

- Molecule 1: Lysostaphin



#### 4.2.15 Score per residue for model 15

- Molecule 1: Lysostaphin



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 15 were deposited, based on the following criterion: *target function*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| CYANA         | structure calculation |         |
| Amber         | refinement            |         |

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

| Chemical shift file(s)                       | working_cs.cif |
|----------------------------------------------|----------------|
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 2622           |
| Number of shifts mapped to atoms             | 2622           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 85%            |

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

| Mol | Chain | Bond lengths |                       | Bond angles |                       |
|-----|-------|--------------|-----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                  | RMSZ        | #Z>5                  |
| 1   | A     | 0.90±0.00    | 0±0/1627 ( 0.0± 0.0%) | 1.40±0.02   | 4±2/2205 ( 0.2± 0.1%) |
| All | All   | 0.90         | 0/24405 ( 0.0%)       | 1.40        | 55/33075 ( 0.2%)      |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 0.7±1.2   |
| All | All   | 0         | 10        |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
|     |       |     |      |           |       |             |          | Worst  | Total |
| 1   | A     | 370 | PHE  | CA-CB-CG  | 7.46  | 121.26      | 113.80   | 14     | 2     |
| 1   | A     | 377 | ASP  | CA-CB-CG  | 7.39  | 119.99      | 112.60   | 5      | 3     |
| 1   | A     | 372 | ASN  | CA-CB-CG  | 6.52  | 119.12      | 112.60   | 6      | 2     |
| 1   | A     | 314 | ILE  | CA-C-N    | 6.48  | 127.06      | 122.33   | 8      | 3     |
| 1   | A     | 314 | ILE  | C-N-CA    | 6.48  | 127.06      | 122.33   | 8      | 3     |
| 1   | A     | 423 | ASP  | CA-CB-CG  | 6.40  | 119.00      | 112.60   | 9      | 2     |
| 1   | A     | 405 | ASN  | CA-CB-CG  | 6.39  | 118.99      | 112.60   | 14     | 1     |
| 1   | A     | 260 | ASN  | CA-CB-CG  | 6.37  | 118.97      | 112.60   | 14     | 1     |
| 1   | A     | 362 | HIS  | CB-CG-CD2 | -6.33 | 122.97      | 131.20   | 2      | 9     |
| 1   | A     | 259 | ASN  | CA-C-N    | 6.33  | 131.66      | 121.98   | 14     | 1     |
| 1   | A     | 259 | ASN  | C-N-CA    | 6.33  | 131.66      | 121.98   | 14     | 1     |
| 1   | A     | 283 | ASP  | CA-CB-CG  | 6.12  | 118.72      | 112.60   | 12     | 5     |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
|     |       |     |      |            |       |             |          | Worst  | Total |
| 1   | A     | 360 | HIS  | CA-CB-CG   | 6.09  | 119.89      | 113.80   | 4      | 3     |
| 1   | A     | 320 | ASP  | CA-CB-CG   | 5.96  | 118.56      | 112.60   | 9      | 2     |
| 1   | A     | 319 | ASN  | CA-CB-CG   | 5.91  | 118.51      | 112.60   | 13     | 1     |
| 1   | A     | 432 | PHE  | CA-CB-CG   | 5.66  | 119.46      | 113.80   | 2      | 3     |
| 1   | A     | 323 | HIS  | CB-CG-CD2  | -5.64 | 123.86      | 131.20   | 14     | 4     |
| 1   | A     | 483 | ASN  | CA-CB-CG   | 5.60  | 118.20      | 112.60   | 6      | 1     |
| 1   | A     | 450 | ASP  | CA-CB-CG   | 5.53  | 118.13      | 112.60   | 2      | 1     |
| 1   | A     | 483 | ASN  | CB-CA-C    | 5.49  | 119.69      | 111.89   | 15     | 1     |
| 1   | A     | 253 | HIS  | CB-CG-CD2  | -5.44 | 124.13      | 131.20   | 4      | 1     |
| 1   | A     | 448 | HIS  | CA-CB-CG   | 5.41  | 119.20      | 113.80   | 8      | 2     |
| 1   | A     | 260 | ASN  | N-CA-CB    | -5.29 | 104.00      | 110.98   | 14     | 1     |
| 1   | A     | 360 | HIS  | CB-CG-CD2  | -5.18 | 124.47      | 131.20   | 15     | 1     |
| 1   | A     | 364 | GLN  | OE1-CD-NE2 | -5.08 | 117.52      | 122.60   | 10     | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 365 | ARG  | Sidechain | 3              |
| 1   | A     | 433 | ARG  | Sidechain | 2              |
| 1   | A     | 470 | ARG  | Sidechain | 2              |
| 1   | A     | 261 | TYR  | Sidechain | 1              |
| 1   | A     | 333 | TYR  | Sidechain | 1              |
| 1   | A     | 387 | TYR  | Sidechain | 1              |

## 6.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 1579  | 1538     | 1538     | 0±1     |
| All | All   | 23700 | 23070    | 23070    | 5       |

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 0.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:402:TRP:CH2 | 1:A:454:LYS:HE3 | 0.49     | 2.43        | 5      | 1     |
| 1:A:402:TRP:CZ2 | 1:A:412:LYS:HE2 | 0.49     | 2.43        | 12     | 1     |
| 1:A:402:TRP:CE2 | 1:A:412:LYS:HE3 | 0.44     | 2.48        | 4      | 1     |
| 1:A:332:LYS:HE3 | 1:A:349:TRP:CZ3 | 0.43     | 2.47        | 5      | 1     |
| 1:A:402:TRP:CZ2 | 1:A:412:LYS:HE3 | 0.43     | 2.48        | 5      | 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     | 197/245 (80%)   | 190±1 (96±1%) | 7±1 (3±1%) | 1±1 (0±0%) | 37          | 78 |
| All | All   | 2955/3675 (80%) | 2848 (96%)    | 99 (3%)    | 8 (0%)     | 37          | 78 |

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 368 | ASN  | 3              |
| 1   | A     | 319 | ASN  | 1              |
| 1   | A     | 388 | GLY  | 1              |
| 1   | A     | 253 | HIS  | 1              |
| 1   | A     | 350 | SER  | 1              |
| 1   | A     | 259 | ASN  | 1              |

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

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

| Mol | Chain | Analysed        | Rotameric     | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|------------|-------------|----|
| 1   | A     | 167/199 (84%)   | 160±3 (96±2%) | 7±3 (4±2%) | 27          | 77 |
| All | All   | 2505/2985 (84%) | 2394 (96%)    | 111 (4%)   | 27          | 77 |

All 39 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     | 433 | ARG  | 14             |
| 1   | A     | 441 | LEU  | 13             |
| 1   | A     | 488 | LEU  | 11             |
| 1   | A     | 367 | VAL  | 7              |
| 1   | A     | 451 | GLU  | 5              |
| 1   | A     | 404 | THR  | 5              |
| 1   | A     | 473 | LEU  | 4              |
| 1   | A     | 319 | ASN  | 4              |
| 1   | A     | 324 | ARG  | 3              |
| 1   | A     | 446 | THR  | 3              |
| 1   | A     | 293 | LYS  | 3              |
| 1   | A     | 301 | VAL  | 3              |
| 1   | A     | 450 | ASP  | 2              |
| 1   | A     | 326 | TRP  | 2              |
| 1   | A     | 332 | LYS  | 2              |
| 1   | A     | 482 | THR  | 2              |
| 1   | A     | 483 | ASN  | 2              |
| 1   | A     | 365 | ARG  | 2              |
| 1   | A     | 370 | PHE  | 2              |
| 1   | A     | 410 | LEU  | 2              |
| 1   | A     | 442 | LYS  | 2              |
| 1   | A     | 333 | TYR  | 1              |
| 1   | A     | 282 | VAL  | 1              |
| 1   | A     | 360 | HIS  | 1              |
| 1   | A     | 376 | GLN  | 1              |
| 1   | A     | 262 | LYS  | 1              |
| 1   | A     | 325 | GLN  | 1              |
| 1   | A     | 342 | LYS  | 1              |
| 1   | A     | 371 | SER  | 1              |
| 1   | A     | 372 | ASN  | 1              |
| 1   | A     | 256 | GLN  | 1              |
| 1   | A     | 313 | GLN  | 1              |
| 1   | A     | 320 | ASP  | 1              |
| 1   | A     | 350 | SER  | 1              |
| 1   | A     | 341 | VAL  | 1              |
| 1   | A     | 368 | ASN  | 1              |
| 1   | A     | 263 | LYS  | 1              |
| 1   | A     | 379 | MET  | 1              |
| 1   | A     | 323 | HIS  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

## 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 85% for the well-defined parts and 82% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *LSSv3.1.bmrB*

#### 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                  | 2622 |
| Number of shifts mapped to atoms        | 2622 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 25   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 235      | $-1.16 \pm 0.17$                | Should be checked          |
| $^{13}\text{C}_\beta$  | 206      | $-1.53 \pm 0.07$                | Should be checked          |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 207      | $0.05 \pm 0.27$                 | 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 85%, i.e. 2275 atoms were assigned a chemical shift out of a possible 2683. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|---------------|-----------------|-----------------|
| Backbone  | 791/999 (79%)   | 407/412 (99%) | 198/396 (50%)   | 186/191 (97%)   |
| Sidechain | 1244/1357 (92%) | 848/885 (96%) | 373/419 (89%)   | 23/53 (43%)     |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 240/327 (73%)   | 143/161 (89%)        | 87/151 (58%)          | 10/15 (67%)           |
| Overall  | 2275/2683 (85%) | 1398/1458 (96%)      | 658/966 (68%)         | 219/259 (85%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 2622 atoms were assigned a chemical shift out of a possible 3187. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 918/1237 (74%)  | 476/514 (93%)        | 235/490 (48%)         | 207/233 (89%)         |
| Sidechain | 1434/1577 (91%) | 976/1028 (95%)       | 431/489 (88%)         | 27/60 (45%)           |
| Aromatic  | 270/373 (72%)   | 162/183 (89%)        | 97/173 (56%)          | 11/17 (65%)           |
| Overall   | 2622/3187 (82%) | 1614/1725 (94%)      | 763/1152 (66%)        | 245/310 (79%)         |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 454 | LYS  | HB3  | -1.02      | 0.46 – 3.04         | -10.8   |
| 1       | A     | 454 | LYS  | HE3  | 0.98       | 1.92 – 3.89         | -9.8    |
| 1       | A     | 454 | LYS  | HD3  | -0.36      | 0.54 – 2.65         | -9.3    |
| 1       | A     | 293 | LYS  | HB3  | -0.64      | 0.46 – 3.04         | -9.3    |
| 1       | A     | 449 | TYR  | CD1  | 120.26     | 125.84 – 139.60     | -9.1    |
| 1       | A     | 454 | LYS  | HD2  | 0.10       | 0.58 – 2.64         | -7.3    |
| 1       | A     | 324 | ARG  | HD3  | 1.30       | 1.81 – 4.39         | -7.0    |
| 1       | A     | 454 | LYS  | HE2  | 1.59       | 1.95 – 3.88         | -6.8    |
| 1       | A     | 474 | PRO  | HB3  | -0.39      | 0.25 – 3.76         | -6.8    |
| 1       | A     | 258 | LEU  | HG   | -0.71      | -0.13 – 3.16        | -6.7    |
| 1       | A     | 372 | ASN  | HB3  | 0.59       | 1.12 – 4.38         | -6.6    |
| 1       | A     | 412 | LYS  | HD3  | 0.25       | 0.54 – 2.65         | -6.4    |
| 1       | A     | 431 | PRO  | HA   | 2.39       | 2.78 – 6.00         | -6.2    |
| 1       | A     | 258 | LEU  | HD21 | -0.96      | -0.65 – 2.13        | -6.1    |
| 1       | A     | 258 | LEU  | HD22 | -0.96      | -0.65 – 2.13        | -6.1    |
| 1       | A     | 258 | LEU  | HD23 | -0.96      | -0.65 – 2.13        | -6.1    |
| 1       | A     | 324 | ARG  | HB3  | 0.16       | 0.43 – 3.11         | -6.0    |
| 1       | A     | 315 | GLY  | HA2  | 6.13       | 2.15 – 5.77         | 6.0     |
| 1       | A     | 324 | ARG  | HB2  | 0.29       | 0.52 – 3.08         | -5.9    |
| 1       | A     | 412 | LYS  | HD2  | 0.40       | 0.58 – 2.64         | -5.8    |
| 1       | A     | 454 | LYS  | HB2  | 0.45       | 0.58 – 2.97         | -5.6    |
| 1       | A     | 293 | LYS  | H    | 4.94       | 5.24 – 11.12        | -5.5    |

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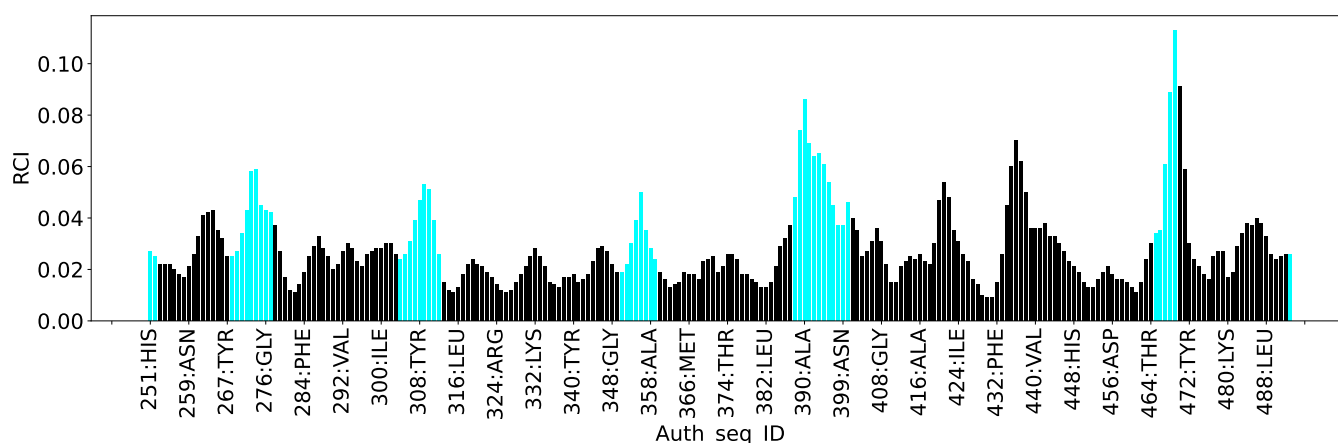
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| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 431 | PRO  | HB3  | 0.09       | 0.25 – 3.76         | -5.5    |
| 1       | A     | 431 | PRO  | HB2  | 0.26       | 0.37 – 3.78         | -5.3    |
| 1       | A     | 324 | ARG  | HD2  | 1.97       | 1.97 – 4.26         | -5.0    |

### 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                                | 3569  |
| Intra-residue ( $ i-j =0$ )                              | 656   |
| Sequential ( $ i-j =1$ )                                 | 821   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 392   |
| Long range ( $ i-j \geq 5$ )                             | 1628  |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 66    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 277   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 15.6  |
| Number of long range restraints per residue <sup>1</sup> | 6.9   |

<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)  | 18.9                                   | 0.2     |
| 0.2-0.5 (Medium) | 15.5                                   | 0.5     |
| >0.5 (Large)     | 1.6                                    | 1.63    |

### 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)   | 18.6                                   | 9.94    |
| 10.0-20.0 (Medium) | 7.7                                    | 19.99   |
| >20.0 (Large)      | 4.3                                    | 127.09  |

## 9 Distance violation analysis ⓘ

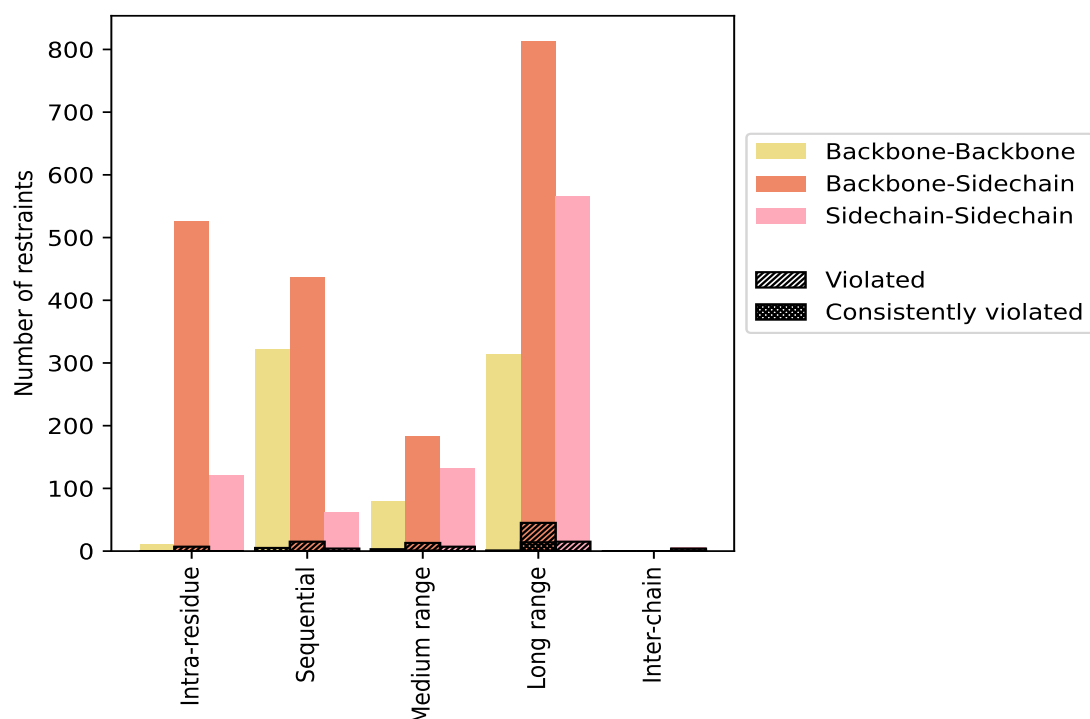
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                             | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                     | Consistently Violated <sup>4</sup> |                      |                     |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|----------------------|---------------------|------------------------------------|----------------------|---------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>      | Count                              | % <sup>2</sup>       | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">656</a>  | <a href="#">18.4</a>  | <a href="#">7</a>     | <a href="#">1.1</a>  | <a href="#">0.2</a> | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 11                   | 0.3                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 525                  | 14.7                  | 7                     | 1.3                  | 0.2                 | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 120                  | 3.4                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">821</a>  | <a href="#">23.0</a>  | <a href="#">24</a>    | <a href="#">2.9</a>  | <a href="#">0.7</a> | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 322                  | 9.0                   | 5                     | 1.6                  | 0.1                 | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 437                  | 12.2                  | 15                    | 3.4                  | 0.4                 | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 62                   | 1.7                   | 4                     | 6.5                  | 0.1                 | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">392</a>  | <a href="#">11.0</a>  | <a href="#">21</a>    | <a href="#">5.4</a>  | <a href="#">0.6</a> | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 80                   | 2.2                   | 3                     | 3.8                  | 0.1                 | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 180                  | 5.0                   | 11                    | 6.1                  | 0.3                 | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 132                  | 3.7                   | 7                     | 5.3                  | 0.2                 | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">1628</a> | <a href="#">45.6</a>  | <a href="#">42</a>    | <a href="#">2.6</a>  | <a href="#">1.2</a> | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 313                  | 8.8                   | 1                     | 0.3                  | 0.0                 | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 750                  | 21.0                  | 26                    | 3.5                  | 0.7                 | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 565                  | 15.8                  | 15                    | 2.7                  | 0.4                 | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">66</a>   | <a href="#">1.8</a>   | <a href="#">21</a>    | <a href="#">31.8</a> | <a href="#">0.6</a> | <a href="#">15</a>                 | <a href="#">22.7</a> | <a href="#">0.4</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">3569</a> | <a href="#">100.0</a> | <a href="#">119</a>   | <a href="#">3.3</a>  | <a href="#">3.3</a> | <a href="#">16</a>                 | <a href="#">0.4</a>  | <a href="#">0.4</a> |
| Backbone-Backbone                                          | 726                  | 20.3                  | 9                     | 1.2                  | 0.3                 | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 1958                 | 54.9                  | 80                    | 4.1                  | 2.2                 | 15                                 | 0.8                  | 0.4                 |
| Sidechain-Sidechain                                        | 885                  | 24.8                  | 30                    | 3.4                  | 0.8                 | 1                                  | 0.1                  | 0.0                 |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 1                    | 4               | 3               | 27              | 3               | 38    | 0.22     | 0.48    | 0.08                | 0.21       |
| 2        | 3                    | 2               | 5               | 25              | 2               | 37    | 0.21     | 0.66    | 0.11                | 0.17       |
| 3        | 1                    | 4               | 5               | 30              | 4               | 44    | 0.23     | 0.9     | 0.14                | 0.2        |
| 4        | 1                    | 4               | 6               | 29              | 3               | 43    | 0.23     | 0.59    | 0.12                | 0.19       |
| 5        | 2                    | 1               | 4               | 23              | 3               | 33    | 0.22     | 1.29    | 0.2                 | 0.18       |
| 6        | 0                    | 2               | 7               | 24              | 3               | 36    | 0.3      | 1.29    | 0.27                | 0.2        |
| 7        | 0                    | 5               | 5               | 29              | 3               | 42    | 0.27     | 1.54    | 0.22                | 0.2        |
| 8        | 1                    | 2               | 8               | 22              | 3               | 36    | 0.25     | 1.5     | 0.22                | 0.2        |
| 9        | 0                    | 2               | 9               | 22              | 3               | 36    | 0.2      | 0.32    | 0.07                | 0.2        |
| 10       | 1                    | 4               | 3               | 28              | 3               | 39    | 0.22     | 0.62    | 0.11                | 0.19       |

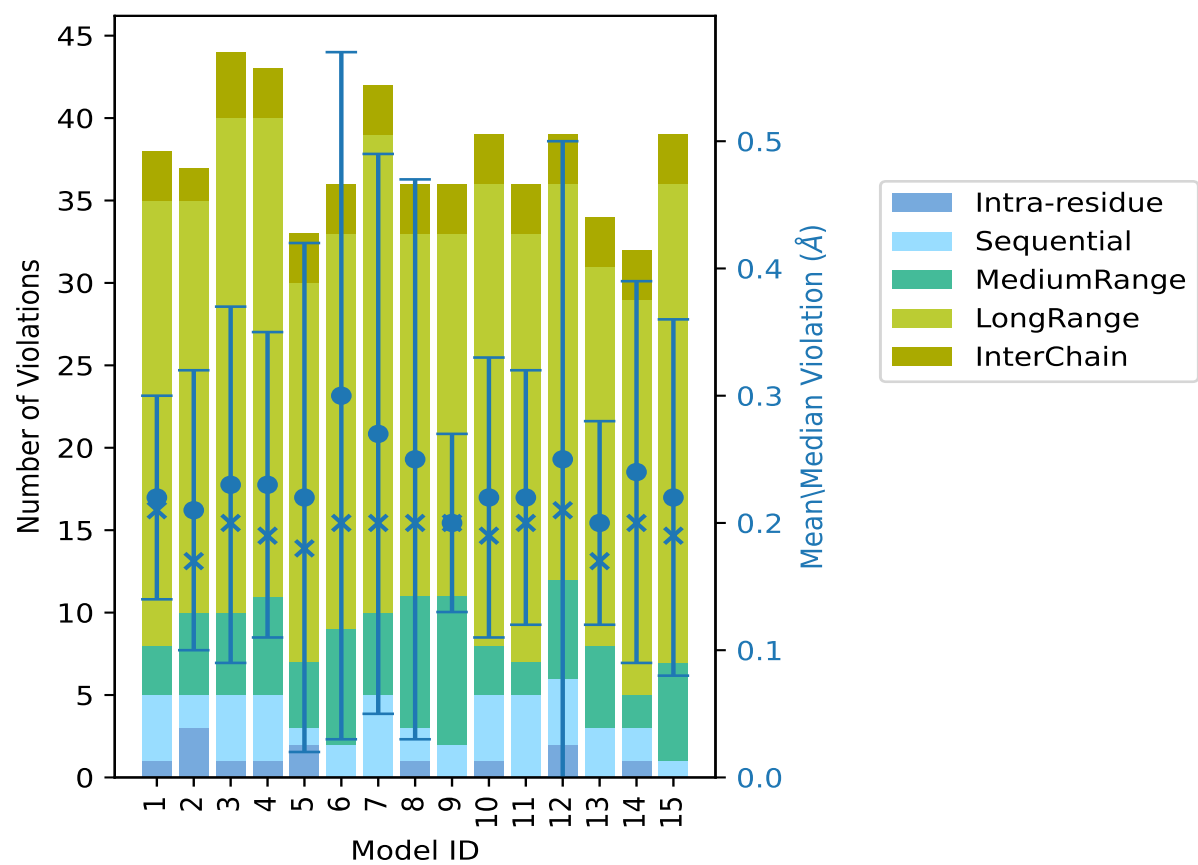
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 0                    | 5               | 2               | 26              | 3               | 36    | 0.22     | 0.66    | 0.1                 | 0.2        |
| 12       | 2                    | 4               | 6               | 24              | 3               | 39    | 0.25     | 1.63    | 0.25                | 0.21       |
| 13       | 0                    | 3               | 5               | 23              | 3               | 34    | 0.2      | 0.51    | 0.08                | 0.17       |
| 14       | 1                    | 2               | 2               | 24              | 3               | 32    | 0.24     | 0.89    | 0.15                | 0.2        |
| 15       | 0                    | 1               | 6               | 29              | 3               | 39    | 0.22     | 0.77    | 0.14                | 0.19       |

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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, 3403(IR:649, SQ:797, MR:371, LR:1586, IC:0) restraints are not violated in the ensemble.

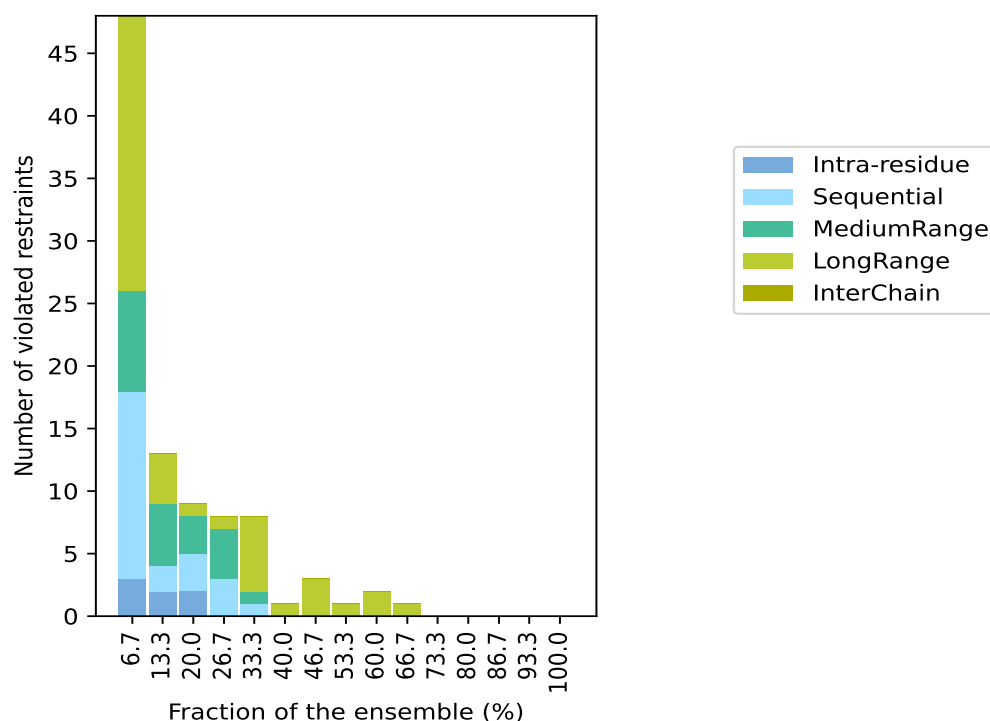
| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 3                             | 15              | 8               | 22              | 0               | 48    | 1                        | 6.7   |
| 2                             | 2               | 5               | 4               | 0               | 13    | 2                        | 13.3  |
| 2                             | 3               | 3               | 1               | 0               | 9     | 3                        | 20.0  |
| 0                             | 3               | 4               | 1               | 0               | 8     | 4                        | 26.7  |
| 0                             | 1               | 1               | 6               | 0               | 8     | 5                        | 33.3  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 6                        | 40.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 7                        | 46.7  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 8                        | 53.3  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 9                        | 60.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 10                       | 66.7  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 73.3  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 12                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 13                       | 86.7  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 14                       | 93.3  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 15                       | 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



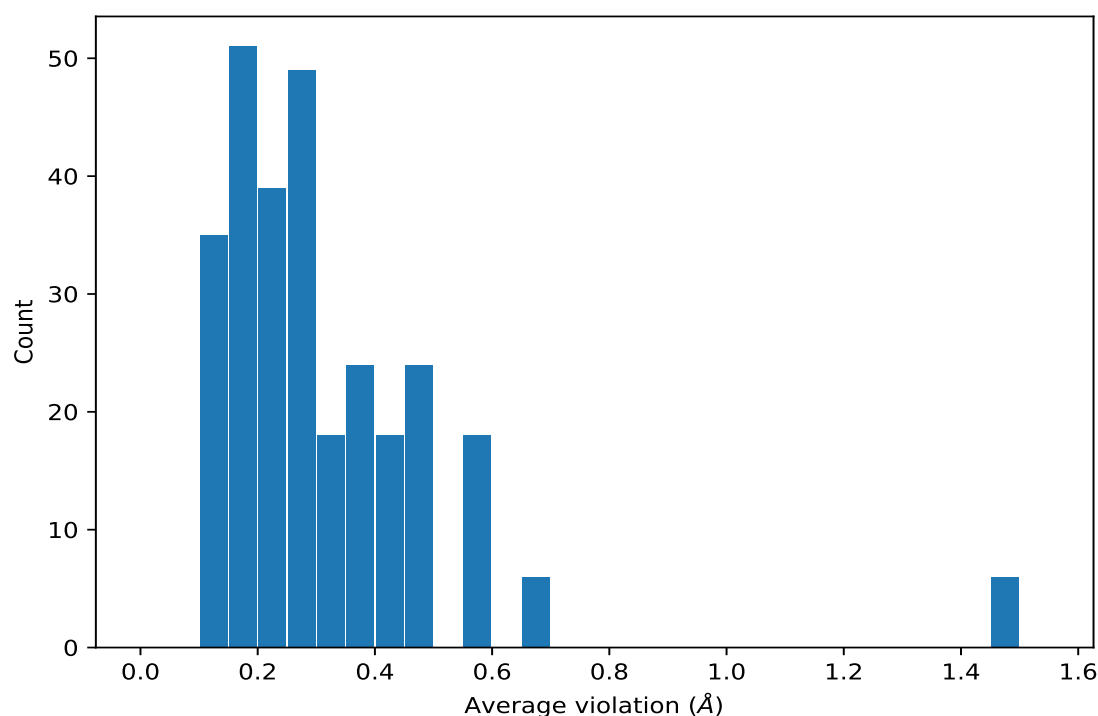
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|--------|-----------------|---------------|---------------------|----------|---------------------|------------|
| (4,20) | 1:473:A:LEU:N   | 1:461:A:VAL:O | 15                  | 0.3      | 0.01                | 0.31       |
| (2,3)  | 1:362:A:HIS:ND1 | 2:501:A:ZN:ZN | 15                  | 0.3      | 0.04                | 0.3        |
| (4,8)  | 1:314:A:ILE:O   | 1:327:A:TYR:N | 15                  | 0.27     | 0.04                | 0.28       |
| (4,3)  | 1:364:A:GLN:N   | 1:326:A:TRP:O | 15                  | 0.27     | 0.03                | 0.28       |
| (4,14) | 1:350:A:SER:N   | 1:290:A:THR:O | 15                  | 0.26     | 0.06                | 0.28       |
| (4,9)  | 1:316:A:LEU:N   | 1:325:A:GLN:O | 15                  | 0.25     | 0.04                | 0.26       |
| (4,11) | 1:299:A:LYS:N   | 1:317:A:ILE:O | 15                  | 0.25     | 0.05                | 0.25       |
| (4,1)  | 1:282:A:VAL:N   | 1:363:A:PHE:O | 15                  | 0.22     | 0.03                | 0.21       |
| (4,2)  | 1:282:A:VAL:O   | 1:363:A:PHE:N | 15                  | 0.22     | 0.03                | 0.22       |
| (4,18) | 1:424:A:ILE:N   | 1:441:A:LEU:O | 15                  | 0.19     | 0.02                | 0.19       |
| (4,4)  | 1:364:A:GLN:O   | 1:326:A:TRP:N | 15                  | 0.19     | 0.03                | 0.19       |
| (4,15) | 1:383:A:LYS:N   | 1:380:A:PRO:O | 15                  | 0.19     | 0.04                | 0.19       |
| (4,7)  | 1:314:A:ILE:N   | 1:327:A:TYR:O | 15                  | 0.18     | 0.04                | 0.17       |
| (4,5)  | 1:366:A:MET:N   | 1:324:A:ARG:O | 15                  | 0.17     | 0.05                | 0.16       |
| (4,12) | 1:299:A:LYS:O   | 1:317:A:ILE:N | 15                  | 0.16     | 0.04                | 0.15       |
| (4,13) | 1:348:A:GLY:O   | 1:292:A:VAL:N | 15                  | 0.13     | 0.02                | 0.14       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (4,6)    | 1:366:A:MET:O    | 1:324:A:ARG:N    | 14                  | 0.19     | 0.04                | 0.18       |
| (2,1)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 14                  | 0.15     | 0.03                | 0.15       |
| (2,6)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 14                  | 0.11     | 0.0                 | 0.11       |
| (4,21)   | 1:471:A:ILE:N    | 1:463:A:TYR:O    | 13                  | 0.18     | 0.05                | 0.2        |
| (4,51)   | 1:383:A:LYS:H    | 1:380:A:PRO:O    | 13                  | 0.14     | 0.02                | 0.14       |
| (4,10)   | 1:316:A:LEU:O    | 1:325:A:GLN:N    | 11                  | 0.14     | 0.03                | 0.14       |
| (1,1997) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HE1  | 10                  | 0.57     | 0.23                | 0.6        |
| (1,1997) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HE1  | 10                  | 0.57     | 0.23                | 0.6        |
| (1,1997) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HE1  | 10                  | 0.57     | 0.23                | 0.6        |
| (1,1997) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HE1  | 10                  | 0.57     | 0.23                | 0.6        |
| (1,1997) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HE1  | 10                  | 0.57     | 0.23                | 0.6        |
| (1,1997) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HE1  | 10                  | 0.57     | 0.23                | 0.6        |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD11 | 9                   | 0.25     | 0.09                | 0.26       |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD12 | 9                   | 0.25     | 0.09                | 0.26       |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD13 | 9                   | 0.25     | 0.09                | 0.26       |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD21 | 9                   | 0.25     | 0.09                | 0.26       |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD22 | 9                   | 0.25     | 0.09                | 0.26       |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD23 | 9                   | 0.25     | 0.09                | 0.26       |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD11 | 9                   | 0.25     | 0.09                | 0.26       |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD12 | 9                   | 0.25     | 0.09                | 0.26       |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD13 | 9                   | 0.25     | 0.09                | 0.26       |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD21 | 9                   | 0.25     | 0.09                | 0.26       |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD22 | 9                   | 0.25     | 0.09                | 0.26       |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD23 | 9                   | 0.25     | 0.09                | 0.26       |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG11 | 9                   | 0.22     | 0.06                | 0.22       |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG12 | 9                   | 0.22     | 0.06                | 0.22       |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG13 | 9                   | 0.22     | 0.06                | 0.22       |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG21 | 9                   | 0.22     | 0.06                | 0.22       |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG22 | 9                   | 0.22     | 0.06                | 0.22       |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG23 | 9                   | 0.22     | 0.06                | 0.22       |
| (1,872)  | 1:304:A:GLY:H    | 1:314:A:ILE:HB   | 8                   | 0.14     | 0.02                | 0.14       |
| (1,1999) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HZ2  | 7                   | 0.39     | 0.13                | 0.31       |
| (1,1999) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HZ2  | 7                   | 0.39     | 0.13                | 0.31       |
| (1,1999) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HZ2  | 7                   | 0.39     | 0.13                | 0.31       |
| (1,1999) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HZ2  | 7                   | 0.39     | 0.13                | 0.31       |
| (1,1999) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HZ2  | 7                   | 0.39     | 0.13                | 0.31       |
| (1,1999) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HZ2  | 7                   | 0.39     | 0.13                | 0.31       |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD11 | 7                   | 0.19     | 0.06                | 0.18       |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD12 | 7                   | 0.19     | 0.06                | 0.18       |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD13 | 7                   | 0.19     | 0.06                | 0.18       |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD21 | 7                   | 0.19     | 0.06                | 0.18       |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD22 | 7                   | 0.19     | 0.06                | 0.18       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD23 | 7                   | 0.19     | 0.06                | 0.18       |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD11 | 7                   | 0.18     | 0.05                | 0.17       |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD12 | 7                   | 0.18     | 0.05                | 0.17       |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD13 | 7                   | 0.18     | 0.05                | 0.17       |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD21 | 7                   | 0.18     | 0.05                | 0.17       |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD22 | 7                   | 0.18     | 0.05                | 0.17       |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD23 | 7                   | 0.18     | 0.05                | 0.17       |
| (1,437)  | 1:282:A:VAL:HG11 | 1:379:A:MET:HA   | 6                   | 0.23     | 0.08                | 0.18       |
| (1,437)  | 1:282:A:VAL:HG12 | 1:379:A:MET:HA   | 6                   | 0.23     | 0.08                | 0.18       |
| (1,437)  | 1:282:A:VAL:HG13 | 1:379:A:MET:HA   | 6                   | 0.23     | 0.08                | 0.18       |
| (1,437)  | 1:282:A:VAL:HG21 | 1:379:A:MET:HA   | 6                   | 0.23     | 0.08                | 0.18       |
| (1,437)  | 1:282:A:VAL:HG22 | 1:379:A:MET:HA   | 6                   | 0.23     | 0.08                | 0.18       |
| (1,437)  | 1:282:A:VAL:HG23 | 1:379:A:MET:HA   | 6                   | 0.23     | 0.08                | 0.18       |
| (1,1223) | 1:330:A:LEU:HD11 | 1:351:A:GLY:H    | 5                   | 0.41     | 0.14                | 0.41       |
| (1,1223) | 1:330:A:LEU:HD12 | 1:351:A:GLY:H    | 5                   | 0.41     | 0.14                | 0.41       |
| (1,1223) | 1:330:A:LEU:HD13 | 1:351:A:GLY:H    | 5                   | 0.41     | 0.14                | 0.41       |
| (1,1223) | 1:330:A:LEU:HD21 | 1:351:A:GLY:H    | 5                   | 0.41     | 0.14                | 0.41       |
| (1,1223) | 1:330:A:LEU:HD22 | 1:351:A:GLY:H    | 5                   | 0.41     | 0.14                | 0.41       |
| (1,1223) | 1:330:A:LEU:HD23 | 1:351:A:GLY:H    | 5                   | 0.41     | 0.14                | 0.41       |
| (1,1221) | 1:330:A:LEU:HD11 | 1:350:A:SER:HA   | 5                   | 0.33     | 0.1                 | 0.32       |
| (1,1221) | 1:330:A:LEU:HD12 | 1:350:A:SER:HA   | 5                   | 0.33     | 0.1                 | 0.32       |
| (1,1221) | 1:330:A:LEU:HD13 | 1:350:A:SER:HA   | 5                   | 0.33     | 0.1                 | 0.32       |
| (1,1221) | 1:330:A:LEU:HD21 | 1:350:A:SER:HA   | 5                   | 0.33     | 0.1                 | 0.32       |
| (1,1221) | 1:330:A:LEU:HD22 | 1:350:A:SER:HA   | 5                   | 0.33     | 0.1                 | 0.32       |
| (1,1221) | 1:330:A:LEU:HD23 | 1:350:A:SER:HA   | 5                   | 0.33     | 0.1                 | 0.32       |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG11 | 5                   | 0.31     | 0.09                | 0.3        |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG12 | 5                   | 0.31     | 0.09                | 0.3        |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG13 | 5                   | 0.31     | 0.09                | 0.3        |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG21 | 5                   | 0.31     | 0.09                | 0.3        |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG22 | 5                   | 0.31     | 0.09                | 0.3        |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG23 | 5                   | 0.31     | 0.09                | 0.3        |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD11 | 5                   | 0.23     | 0.17                | 0.14       |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD12 | 5                   | 0.23     | 0.17                | 0.14       |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD13 | 5                   | 0.23     | 0.17                | 0.14       |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD21 | 5                   | 0.23     | 0.17                | 0.14       |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD22 | 5                   | 0.23     | 0.17                | 0.14       |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD23 | 5                   | 0.23     | 0.17                | 0.14       |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD11 | 5                   | 0.19     | 0.06                | 0.17       |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD12 | 5                   | 0.19     | 0.06                | 0.17       |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD13 | 5                   | 0.19     | 0.06                | 0.17       |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD21 | 5                   | 0.19     | 0.06                | 0.17       |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD22 | 5                   | 0.19     | 0.06                | 0.17       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD23 | 5                   | 0.19     | 0.06                | 0.17       |
| (1,3467) | 1:492:A:ILE:HD11 | 1:493:A:LYS:H    | 5                   | 0.19     | 0.04                | 0.2        |
| (1,3467) | 1:492:A:ILE:HD12 | 1:493:A:LYS:H    | 5                   | 0.19     | 0.04                | 0.2        |
| (1,3467) | 1:492:A:ILE:HD13 | 1:493:A:LYS:H    | 5                   | 0.19     | 0.04                | 0.2        |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG11 | 5                   | 0.14     | 0.03                | 0.14       |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG12 | 5                   | 0.14     | 0.03                | 0.14       |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG13 | 5                   | 0.14     | 0.03                | 0.14       |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG21 | 5                   | 0.14     | 0.03                | 0.14       |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG22 | 5                   | 0.14     | 0.03                | 0.14       |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG23 | 5                   | 0.14     | 0.03                | 0.14       |
| (1,3333) | 1:478:A:TRP:HD1  | 1:485:A:LEU:HG   | 5                   | 0.12     | 0.01                | 0.12       |
| (4,22)   | 1:461:A:VAL:N    | 1:473:A:LEU:O    | 5                   | 0.11     | 0.01                | 0.12       |
| (1,3414) | 1:487:A:VAL:HG11 | 1:489:A:TRP:HE1  | 4                   | 1.49     | 0.12                | 1.52       |
| (1,3414) | 1:487:A:VAL:HG12 | 1:489:A:TRP:HE1  | 4                   | 1.49     | 0.12                | 1.52       |
| (1,3414) | 1:487:A:VAL:HG13 | 1:489:A:TRP:HE1  | 4                   | 1.49     | 0.12                | 1.52       |
| (1,3414) | 1:487:A:VAL:HG21 | 1:489:A:TRP:HE1  | 4                   | 1.49     | 0.12                | 1.52       |
| (1,3414) | 1:487:A:VAL:HG22 | 1:489:A:TRP:HE1  | 4                   | 1.49     | 0.12                | 1.52       |
| (1,3414) | 1:487:A:VAL:HG23 | 1:489:A:TRP:HE1  | 4                   | 1.49     | 0.12                | 1.52       |
| (1,3425) | 1:488:A:LEU:HD11 | 1:489:A:TRP:HE1  | 4                   | 0.45     | 0.07                | 0.45       |
| (1,3425) | 1:488:A:LEU:HD12 | 1:489:A:TRP:HE1  | 4                   | 0.45     | 0.07                | 0.45       |
| (1,3425) | 1:488:A:LEU:HD13 | 1:489:A:TRP:HE1  | 4                   | 0.45     | 0.07                | 0.45       |
| (1,3425) | 1:488:A:LEU:HD21 | 1:489:A:TRP:HE1  | 4                   | 0.45     | 0.07                | 0.45       |
| (1,3425) | 1:488:A:LEU:HD22 | 1:489:A:TRP:HE1  | 4                   | 0.45     | 0.07                | 0.45       |
| (1,3425) | 1:488:A:LEU:HD23 | 1:489:A:TRP:HE1  | 4                   | 0.45     | 0.07                | 0.45       |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG11 | 4                   | 0.41     | 0.22                | 0.33       |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG12 | 4                   | 0.41     | 0.22                | 0.33       |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG13 | 4                   | 0.41     | 0.22                | 0.33       |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG21 | 4                   | 0.41     | 0.22                | 0.33       |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG22 | 4                   | 0.41     | 0.22                | 0.33       |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG23 | 4                   | 0.41     | 0.22                | 0.33       |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG11 | 4                   | 0.41     | 0.22                | 0.33       |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG12 | 4                   | 0.41     | 0.22                | 0.33       |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG13 | 4                   | 0.41     | 0.22                | 0.33       |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG21 | 4                   | 0.41     | 0.22                | 0.33       |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG22 | 4                   | 0.41     | 0.22                | 0.33       |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG23 | 4                   | 0.41     | 0.22                | 0.33       |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD11 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD12 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD13 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD21 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD22 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD23 | 4                   | 0.36     | 0.06                | 0.34       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD11 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD12 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD13 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD21 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD22 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD23 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD11 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD12 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD13 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD21 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD22 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD23 | 4                   | 0.36     | 0.06                | 0.34       |
| (1,1577) | 1:367:A:VAL:HB   | 1:369:A:SER:H    | 4                   | 0.24     | 0.02                | 0.24       |
| (1,2666) | 1:440:A:VAL:HG11 | 1:442:A:LYS:H    | 4                   | 0.2      | 0.05                | 0.21       |
| (1,2666) | 1:440:A:VAL:HG12 | 1:442:A:LYS:H    | 4                   | 0.2      | 0.05                | 0.21       |
| (1,2666) | 1:440:A:VAL:HG13 | 1:442:A:LYS:H    | 4                   | 0.2      | 0.05                | 0.21       |
| (1,2666) | 1:440:A:VAL:HG21 | 1:442:A:LYS:H    | 4                   | 0.2      | 0.05                | 0.21       |
| (1,2666) | 1:440:A:VAL:HG22 | 1:442:A:LYS:H    | 4                   | 0.2      | 0.05                | 0.21       |
| (1,2666) | 1:440:A:VAL:HG23 | 1:442:A:LYS:H    | 4                   | 0.2      | 0.05                | 0.21       |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG11 | 4                   | 0.19     | 0.02                | 0.2        |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG12 | 4                   | 0.19     | 0.02                | 0.2        |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG13 | 4                   | 0.19     | 0.02                | 0.2        |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG21 | 4                   | 0.19     | 0.02                | 0.2        |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG22 | 4                   | 0.19     | 0.02                | 0.2        |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG23 | 4                   | 0.19     | 0.02                | 0.2        |
| (1,3471) | 1:492:A:ILE:HG21 | 1:493:A:LYS:HG2  | 4                   | 0.15     | 0.01                | 0.15       |
| (1,3471) | 1:492:A:ILE:HG21 | 1:493:A:LYS:HG3  | 4                   | 0.15     | 0.01                | 0.15       |
| (1,3471) | 1:492:A:ILE:HG22 | 1:493:A:LYS:HG2  | 4                   | 0.15     | 0.01                | 0.15       |
| (1,3471) | 1:492:A:ILE:HG22 | 1:493:A:LYS:HG3  | 4                   | 0.15     | 0.01                | 0.15       |
| (1,3471) | 1:492:A:ILE:HG23 | 1:493:A:LYS:HG2  | 4                   | 0.15     | 0.01                | 0.15       |
| (1,3471) | 1:492:A:ILE:HG23 | 1:493:A:LYS:HG3  | 4                   | 0.15     | 0.01                | 0.15       |
| (1,3413) | 1:487:A:VAL:HG11 | 1:489:A:TRP:HD1  | 3                   | 0.46     | 0.09                | 0.42       |
| (1,3413) | 1:487:A:VAL:HG12 | 1:489:A:TRP:HD1  | 3                   | 0.46     | 0.09                | 0.42       |
| (1,3413) | 1:487:A:VAL:HG13 | 1:489:A:TRP:HD1  | 3                   | 0.46     | 0.09                | 0.42       |
| (1,3413) | 1:487:A:VAL:HG21 | 1:489:A:TRP:HD1  | 3                   | 0.46     | 0.09                | 0.42       |
| (1,3413) | 1:487:A:VAL:HG22 | 1:489:A:TRP:HD1  | 3                   | 0.46     | 0.09                | 0.42       |
| (1,3413) | 1:487:A:VAL:HG23 | 1:489:A:TRP:HD1  | 3                   | 0.46     | 0.09                | 0.42       |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG11 | 3                   | 0.27     | 0.04                | 0.25       |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG12 | 3                   | 0.27     | 0.04                | 0.25       |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG13 | 3                   | 0.27     | 0.04                | 0.25       |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG21 | 3                   | 0.27     | 0.04                | 0.25       |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG22 | 3                   | 0.27     | 0.04                | 0.25       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG23 | 3                   | 0.27     | 0.04                | 0.25       |
| (1,3412) | 1:487:A:VAL:HG11 | 1:489:A:TRP:H    | 3                   | 0.27     | 0.08                | 0.23       |
| (1,3412) | 1:487:A:VAL:HG12 | 1:489:A:TRP:H    | 3                   | 0.27     | 0.08                | 0.23       |
| (1,3412) | 1:487:A:VAL:HG13 | 1:489:A:TRP:H    | 3                   | 0.27     | 0.08                | 0.23       |
| (1,3412) | 1:487:A:VAL:HG21 | 1:489:A:TRP:H    | 3                   | 0.27     | 0.08                | 0.23       |
| (1,3412) | 1:487:A:VAL:HG22 | 1:489:A:TRP:H    | 3                   | 0.27     | 0.08                | 0.23       |
| (1,3412) | 1:487:A:VAL:HG23 | 1:489:A:TRP:H    | 3                   | 0.27     | 0.08                | 0.23       |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG11 | 3                   | 0.27     | 0.08                | 0.23       |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG12 | 3                   | 0.27     | 0.08                | 0.23       |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG13 | 3                   | 0.27     | 0.08                | 0.23       |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG21 | 3                   | 0.27     | 0.08                | 0.23       |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG22 | 3                   | 0.27     | 0.08                | 0.23       |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG23 | 3                   | 0.27     | 0.08                | 0.23       |
| (1,1375) | 1:341:A:VAL:HG11 | 1:343:A:ALA:H    | 3                   | 0.23     | 0.05                | 0.23       |
| (1,1375) | 1:341:A:VAL:HG12 | 1:343:A:ALA:H    | 3                   | 0.23     | 0.05                | 0.23       |
| (1,1375) | 1:341:A:VAL:HG13 | 1:343:A:ALA:H    | 3                   | 0.23     | 0.05                | 0.23       |
| (1,1375) | 1:341:A:VAL:HG21 | 1:343:A:ALA:H    | 3                   | 0.23     | 0.05                | 0.23       |
| (1,1375) | 1:341:A:VAL:HG22 | 1:343:A:ALA:H    | 3                   | 0.23     | 0.05                | 0.23       |
| (1,1375) | 1:341:A:VAL:HG23 | 1:343:A:ALA:H    | 3                   | 0.23     | 0.05                | 0.23       |
| (1,1209) | 1:330:A:LEU:HD11 | 1:331:A:SER:H    | 3                   | 0.22     | 0.1                 | 0.19       |
| (1,1209) | 1:330:A:LEU:HD12 | 1:331:A:SER:H    | 3                   | 0.22     | 0.1                 | 0.19       |
| (1,1209) | 1:330:A:LEU:HD13 | 1:331:A:SER:H    | 3                   | 0.22     | 0.1                 | 0.19       |
| (1,1209) | 1:330:A:LEU:HD21 | 1:331:A:SER:H    | 3                   | 0.22     | 0.1                 | 0.19       |
| (1,1209) | 1:330:A:LEU:HD22 | 1:331:A:SER:H    | 3                   | 0.22     | 0.1                 | 0.19       |
| (1,1209) | 1:330:A:LEU:HD23 | 1:331:A:SER:H    | 3                   | 0.22     | 0.1                 | 0.19       |
| (1,2087) | 1:415:A:SER:HB2  | 1:416:A:ALA:H    | 3                   | 0.16     | 0.01                | 0.16       |
| (1,2087) | 1:415:A:SER:HB3  | 1:416:A:ALA:H    | 3                   | 0.16     | 0.01                | 0.16       |
| (1,1474) | 1:357:A:THR:HA   | 1:357:A:THR:HG21 | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,1474) | 1:357:A:THR:HA   | 1:357:A:THR:HG22 | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,1474) | 1:357:A:THR:HA   | 1:357:A:THR:HG23 | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,1780) | 1:397:A:THR:HA   | 1:397:A:THR:HG21 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1780) | 1:397:A:THR:HA   | 1:397:A:THR:HG22 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1780) | 1:397:A:THR:HA   | 1:397:A:THR:HG23 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD11 | 2                   | 0.68     | 0.52                | 0.68       |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD12 | 2                   | 0.68     | 0.52                | 0.68       |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD13 | 2                   | 0.68     | 0.52                | 0.68       |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD21 | 2                   | 0.68     | 0.52                | 0.68       |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD22 | 2                   | 0.68     | 0.52                | 0.68       |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD23 | 2                   | 0.68     | 0.52                | 0.68       |
| (1,1215) | 1:330:A:LEU:HD11 | 1:333:A:TYR:HE1  | 2                   | 0.56     | 0.21                | 0.56       |
| (1,1215) | 1:330:A:LEU:HD11 | 1:333:A:TYR:HE2  | 2                   | 0.56     | 0.21                | 0.56       |
| (1,1215) | 1:330:A:LEU:HD12 | 1:333:A:TYR:HE1  | 2                   | 0.56     | 0.21                | 0.56       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1215) | 1:330:A:LEU:HD12 | 1:333:A:TYR:HE2  | 2                   | 0.56     | 0.21                | 0.56       |
| (1,1215) | 1:330:A:LEU:HD13 | 1:333:A:TYR:HE1  | 2                   | 0.56     | 0.21                | 0.56       |
| (1,1215) | 1:330:A:LEU:HD13 | 1:333:A:TYR:HE2  | 2                   | 0.56     | 0.21                | 0.56       |
| (1,1215) | 1:330:A:LEU:HD21 | 1:333:A:TYR:HE1  | 2                   | 0.56     | 0.21                | 0.56       |
| (1,1215) | 1:330:A:LEU:HD21 | 1:333:A:TYR:HE2  | 2                   | 0.56     | 0.21                | 0.56       |
| (1,1215) | 1:330:A:LEU:HD22 | 1:333:A:TYR:HE1  | 2                   | 0.56     | 0.21                | 0.56       |
| (1,1215) | 1:330:A:LEU:HD22 | 1:333:A:TYR:HE2  | 2                   | 0.56     | 0.21                | 0.56       |
| (1,1215) | 1:330:A:LEU:HD23 | 1:333:A:TYR:HE1  | 2                   | 0.56     | 0.21                | 0.56       |
| (1,1215) | 1:330:A:LEU:HD23 | 1:333:A:TYR:HE2  | 2                   | 0.56     | 0.21                | 0.56       |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG11 | 2                   | 0.46     | 0.09                | 0.46       |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG12 | 2                   | 0.46     | 0.09                | 0.46       |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG13 | 2                   | 0.46     | 0.09                | 0.46       |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG21 | 2                   | 0.46     | 0.09                | 0.46       |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG22 | 2                   | 0.46     | 0.09                | 0.46       |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG23 | 2                   | 0.46     | 0.09                | 0.46       |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG11 | 2                   | 0.46     | 0.09                | 0.46       |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG12 | 2                   | 0.46     | 0.09                | 0.46       |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG13 | 2                   | 0.46     | 0.09                | 0.46       |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG21 | 2                   | 0.46     | 0.09                | 0.46       |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG22 | 2                   | 0.46     | 0.09                | 0.46       |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG23 | 2                   | 0.46     | 0.09                | 0.46       |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG11 | 2                   | 0.32     | 0.12                | 0.32       |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG12 | 2                   | 0.32     | 0.12                | 0.32       |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG13 | 2                   | 0.32     | 0.12                | 0.32       |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG21 | 2                   | 0.32     | 0.12                | 0.32       |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG22 | 2                   | 0.32     | 0.12                | 0.32       |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG23 | 2                   | 0.32     | 0.12                | 0.32       |
| (1,996)  | 1:316:A:LEU:HD11 | 1:318:A:GLU:H    | 2                   | 0.27     | 0.1                 | 0.27       |
| (1,996)  | 1:316:A:LEU:HD12 | 1:318:A:GLU:H    | 2                   | 0.27     | 0.1                 | 0.27       |
| (1,996)  | 1:316:A:LEU:HD13 | 1:318:A:GLU:H    | 2                   | 0.27     | 0.1                 | 0.27       |
| (1,996)  | 1:316:A:LEU:HD21 | 1:318:A:GLU:H    | 2                   | 0.27     | 0.1                 | 0.27       |
| (1,996)  | 1:316:A:LEU:HD22 | 1:318:A:GLU:H    | 2                   | 0.27     | 0.1                 | 0.27       |
| (1,996)  | 1:316:A:LEU:HD23 | 1:318:A:GLU:H    | 2                   | 0.27     | 0.1                 | 0.27       |
| (1,3400) | 1:485:A:LEU:HD11 | 1:486:A:GLY:H    | 2                   | 0.26     | 0.05                | 0.26       |
| (1,3400) | 1:485:A:LEU:HD12 | 1:486:A:GLY:H    | 2                   | 0.26     | 0.05                | 0.26       |
| (1,3400) | 1:485:A:LEU:HD13 | 1:486:A:GLY:H    | 2                   | 0.26     | 0.05                | 0.26       |
| (1,3400) | 1:485:A:LEU:HD21 | 1:486:A:GLY:H    | 2                   | 0.26     | 0.05                | 0.26       |
| (1,3400) | 1:485:A:LEU:HD22 | 1:486:A:GLY:H    | 2                   | 0.26     | 0.05                | 0.26       |
| (1,3400) | 1:485:A:LEU:HD23 | 1:486:A:GLY:H    | 2                   | 0.26     | 0.05                | 0.26       |
| (1,1984) | 1:410:A:LEU:HD11 | 1:411:A:TYR:H    | 2                   | 0.18     | 0.06                | 0.18       |
| (1,1984) | 1:410:A:LEU:HD12 | 1:411:A:TYR:H    | 2                   | 0.18     | 0.06                | 0.18       |
| (1,1984) | 1:410:A:LEU:HD13 | 1:411:A:TYR:H    | 2                   | 0.18     | 0.06                | 0.18       |

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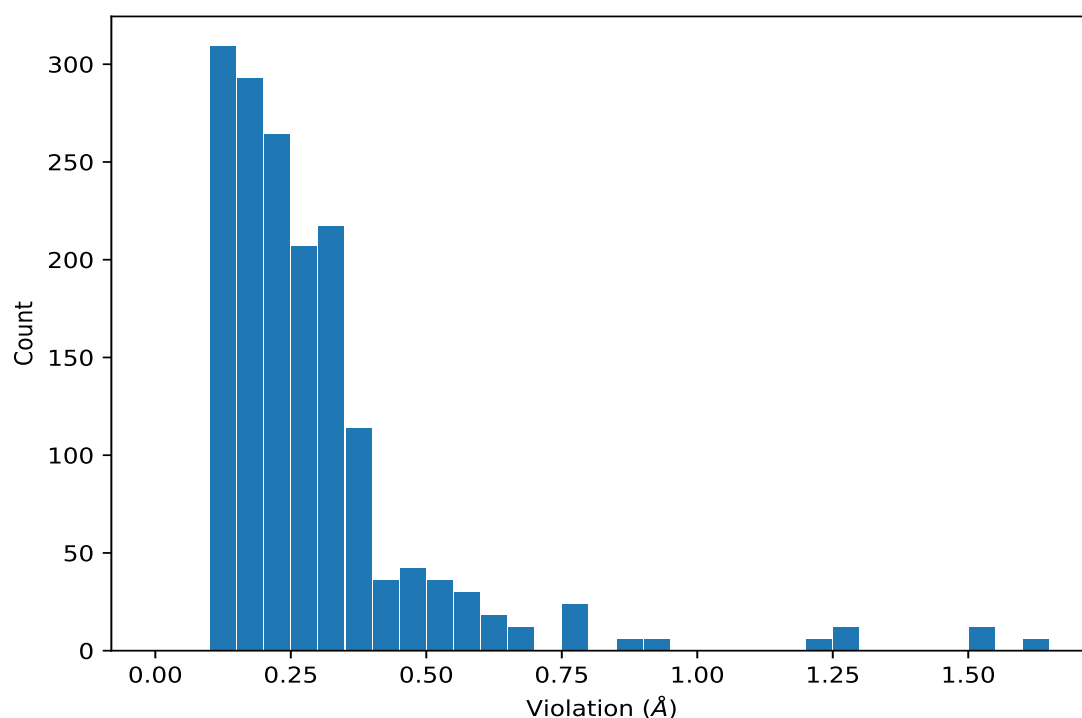
| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1984) | 1:410:A:LEU:HD21 | 1:411:A:TYR:H   | 2                   | 0.18     | 0.06                | 0.18       |
| (1,1984) | 1:410:A:LEU:HD22 | 1:411:A:TYR:H   | 2                   | 0.18     | 0.06                | 0.18       |
| (1,1984) | 1:410:A:LEU:HD23 | 1:411:A:TYR:H   | 2                   | 0.18     | 0.06                | 0.18       |
| (1,2803) | 1:451:A:GLU:HB2  | 1:462:A:GLY:HA3 | 2                   | 0.16     | 0.01                | 0.16       |
| (1,2803) | 1:451:A:GLU:HB3  | 1:462:A:GLY:HA3 | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1378) | 1:341:A:VAL:HG11 | 1:345:A:GLN:H   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1378) | 1:341:A:VAL:HG12 | 1:345:A:GLN:H   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1378) | 1:341:A:VAL:HG13 | 1:345:A:GLN:H   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1378) | 1:341:A:VAL:HG21 | 1:345:A:GLN:H   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1378) | 1:341:A:VAL:HG22 | 1:345:A:GLN:H   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1378) | 1:341:A:VAL:HG23 | 1:345:A:GLN:H   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,379)  | 1:278:A:MET:H    | 1:278:A:MET:HE1 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,379)  | 1:278:A:MET:H    | 1:278:A:MET:HE2 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,379)  | 1:278:A:MET:H    | 1:278:A:MET:HE3 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,3159) | 1:470:A:ARG:H    | 1:470:A:ARG:HD2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,3159) | 1:470:A:ARG:H    | 1:470:A:ARG:HD3 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2446) | 1:426:A:THR:HA   | 1:474:A:PRO:HG3 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1046) | 1:318:A:GLU:HA   | 1:320:A:ASP:H   | 2                   | 0.12     | 0.0                 | 0.12       |
| (4,16)   | 1:453:A:MET:N    | 1:460:A:TRP:O   | 2                   | 0.11     | 0.01                | 0.11       |
| (2,4)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN   | 2                   | 0.1      | 0.0                 | 0.1        |

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

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

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

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



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

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

| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3414) | 1:487:A:VAL:HG11 | 1:489:A:TRP:HE1 | 12       | 1.63          |
| (1,3414) | 1:487:A:VAL:HG12 | 1:489:A:TRP:HE1 | 12       | 1.63          |
| (1,3414) | 1:487:A:VAL:HG13 | 1:489:A:TRP:HE1 | 12       | 1.63          |
| (1,3414) | 1:487:A:VAL:HG21 | 1:489:A:TRP:HE1 | 12       | 1.63          |
| (1,3414) | 1:487:A:VAL:HG22 | 1:489:A:TRP:HE1 | 12       | 1.63          |
| (1,3414) | 1:487:A:VAL:HG23 | 1:489:A:TRP:HE1 | 12       | 1.63          |
| (1,3414) | 1:487:A:VAL:HG11 | 1:489:A:TRP:HE1 | 7        | 1.54          |
| (1,3414) | 1:487:A:VAL:HG12 | 1:489:A:TRP:HE1 | 7        | 1.54          |
| (1,3414) | 1:487:A:VAL:HG13 | 1:489:A:TRP:HE1 | 7        | 1.54          |
| (1,3414) | 1:487:A:VAL:HG21 | 1:489:A:TRP:HE1 | 7        | 1.54          |
| (1,3414) | 1:487:A:VAL:HG22 | 1:489:A:TRP:HE1 | 7        | 1.54          |
| (1,3414) | 1:487:A:VAL:HG23 | 1:489:A:TRP:HE1 | 7        | 1.54          |
| (1,3414) | 1:487:A:VAL:HG11 | 1:489:A:TRP:HE1 | 8        | 1.5           |
| (1,3414) | 1:487:A:VAL:HG12 | 1:489:A:TRP:HE1 | 8        | 1.5           |
| (1,3414) | 1:487:A:VAL:HG13 | 1:489:A:TRP:HE1 | 8        | 1.5           |
| (1,3414) | 1:487:A:VAL:HG21 | 1:489:A:TRP:HE1 | 8        | 1.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3414) | 1:487:A:VAL:HG22 | 1:489:A:TRP:HE1  | 8        | 1.5           |
| (1,3414) | 1:487:A:VAL:HG23 | 1:489:A:TRP:HE1  | 8        | 1.5           |
| (1,3414) | 1:487:A:VAL:HG11 | 1:489:A:TRP:HE1  | 5        | 1.29          |
| (1,3414) | 1:487:A:VAL:HG12 | 1:489:A:TRP:HE1  | 5        | 1.29          |
| (1,3414) | 1:487:A:VAL:HG13 | 1:489:A:TRP:HE1  | 5        | 1.29          |
| (1,3414) | 1:487:A:VAL:HG21 | 1:489:A:TRP:HE1  | 5        | 1.29          |
| (1,3414) | 1:487:A:VAL:HG22 | 1:489:A:TRP:HE1  | 5        | 1.29          |
| (1,3414) | 1:487:A:VAL:HG23 | 1:489:A:TRP:HE1  | 5        | 1.29          |
| (1,930)  | 1:313:A:GLN:HA   | 1:330:A:LEU:HD11 | 6        | 1.29          |
| (1,930)  | 1:313:A:GLN:HA   | 1:330:A:LEU:HD12 | 6        | 1.29          |
| (1,930)  | 1:313:A:GLN:HA   | 1:330:A:LEU:HD13 | 6        | 1.29          |
| (1,930)  | 1:313:A:GLN:HA   | 1:330:A:LEU:HD21 | 6        | 1.29          |
| (1,930)  | 1:313:A:GLN:HA   | 1:330:A:LEU:HD22 | 6        | 1.29          |
| (1,930)  | 1:313:A:GLN:HA   | 1:330:A:LEU:HD23 | 6        | 1.29          |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD11 | 6        | 1.2           |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD12 | 6        | 1.2           |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD13 | 6        | 1.2           |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD21 | 6        | 1.2           |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD22 | 6        | 1.2           |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD23 | 6        | 1.2           |
| (1,1997) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HE1  | 3        | 0.9           |
| (1,1997) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HE1  | 3        | 0.9           |
| (1,1997) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HE1  | 3        | 0.9           |
| (1,1997) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HE1  | 3        | 0.9           |
| (1,1997) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HE1  | 3        | 0.9           |
| (1,1997) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HE1  | 3        | 0.9           |
| (1,1997) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HE1  | 14       | 0.89          |
| (1,1997) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HE1  | 14       | 0.89          |
| (1,1997) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HE1  | 14       | 0.89          |
| (1,1997) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HE1  | 14       | 0.89          |
| (1,1997) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HE1  | 14       | 0.89          |
| (1,1997) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HE1  | 14       | 0.89          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG11 | 15       | 0.77          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG12 | 15       | 0.77          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG13 | 15       | 0.77          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG21 | 15       | 0.77          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG22 | 15       | 0.77          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG23 | 15       | 0.77          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG11 | 15       | 0.77          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG12 | 15       | 0.77          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG13 | 15       | 0.77          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG21 | 15       | 0.77          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG22 | 15       | 0.77          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG23 | 15       | 0.77          |
| (1,1215) | 1:330:A:LEU:HD11 | 1:333:A:TYR:HE1  | 6        | 0.77          |
| (1,1215) | 1:330:A:LEU:HD11 | 1:333:A:TYR:HE2  | 6        | 0.77          |
| (1,1215) | 1:330:A:LEU:HD12 | 1:333:A:TYR:HE1  | 6        | 0.77          |
| (1,1215) | 1:330:A:LEU:HD12 | 1:333:A:TYR:HE2  | 6        | 0.77          |
| (1,1215) | 1:330:A:LEU:HD13 | 1:333:A:TYR:HE1  | 6        | 0.77          |
| (1,1215) | 1:330:A:LEU:HD13 | 1:333:A:TYR:HE2  | 6        | 0.77          |
| (1,1215) | 1:330:A:LEU:HD21 | 1:333:A:TYR:HE1  | 6        | 0.77          |
| (1,1215) | 1:330:A:LEU:HD21 | 1:333:A:TYR:HE2  | 6        | 0.77          |
| (1,1215) | 1:330:A:LEU:HD22 | 1:333:A:TYR:HE1  | 6        | 0.77          |
| (1,1215) | 1:330:A:LEU:HD22 | 1:333:A:TYR:HE2  | 6        | 0.77          |
| (1,1215) | 1:330:A:LEU:HD23 | 1:333:A:TYR:HE1  | 6        | 0.77          |
| (1,1215) | 1:330:A:LEU:HD23 | 1:333:A:TYR:HE2  | 6        | 0.77          |
| (1,1997) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HE1  | 2        | 0.66          |
| (1,1997) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HE1  | 2        | 0.66          |
| (1,1997) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HE1  | 2        | 0.66          |
| (1,1997) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HE1  | 2        | 0.66          |
| (1,1997) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HE1  | 2        | 0.66          |
| (1,1997) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HE1  | 2        | 0.66          |
| (1,1997) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HE1  | 11       | 0.66          |
| (1,1997) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HE1  | 11       | 0.66          |
| (1,1997) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HE1  | 11       | 0.66          |
| (1,1997) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HE1  | 11       | 0.66          |
| (1,1997) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HE1  | 11       | 0.66          |
| (1,1997) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HE1  | 11       | 0.66          |
| (1,1999) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HZ2  | 3        | 0.62          |
| (1,1999) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HZ2  | 3        | 0.62          |
| (1,1999) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HZ2  | 3        | 0.62          |
| (1,1999) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HZ2  | 3        | 0.62          |
| (1,1999) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HZ2  | 3        | 0.62          |
| (1,1999) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HZ2  | 3        | 0.62          |
| (1,1223) | 1:330:A:LEU:HD11 | 1:351:A:GLY:H    | 10       | 0.62          |
| (1,1223) | 1:330:A:LEU:HD12 | 1:351:A:GLY:H    | 10       | 0.62          |
| (1,1223) | 1:330:A:LEU:HD13 | 1:351:A:GLY:H    | 10       | 0.62          |
| (1,1223) | 1:330:A:LEU:HD21 | 1:351:A:GLY:H    | 10       | 0.62          |
| (1,1223) | 1:330:A:LEU:HD22 | 1:351:A:GLY:H    | 10       | 0.62          |
| (1,1223) | 1:330:A:LEU:HD23 | 1:351:A:GLY:H    | 10       | 0.62          |
| (1,1997) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HE1  | 15       | 0.6           |
| (1,1997) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HE1  | 15       | 0.6           |
| (1,1997) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HE1  | 15       | 0.6           |
| (1,1997) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HE1  | 15       | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1997) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HE1  | 15       | 0.6           |
| (1,1997) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HE1  | 15       | 0.6           |
| (1,3413) | 1:487:A:VAL:HG11 | 1:489:A:TRP:HD1  | 12       | 0.59          |
| (1,3413) | 1:487:A:VAL:HG12 | 1:489:A:TRP:HD1  | 12       | 0.59          |
| (1,3413) | 1:487:A:VAL:HG13 | 1:489:A:TRP:HD1  | 12       | 0.59          |
| (1,3413) | 1:487:A:VAL:HG21 | 1:489:A:TRP:HD1  | 12       | 0.59          |
| (1,3413) | 1:487:A:VAL:HG22 | 1:489:A:TRP:HD1  | 12       | 0.59          |
| (1,3413) | 1:487:A:VAL:HG23 | 1:489:A:TRP:HD1  | 12       | 0.59          |
| (1,1997) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HE1  | 4        | 0.59          |
| (1,1997) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HE1  | 4        | 0.59          |
| (1,1997) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HE1  | 4        | 0.59          |
| (1,1997) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HE1  | 4        | 0.59          |
| (1,1997) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HE1  | 4        | 0.59          |
| (1,1997) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HE1  | 4        | 0.59          |
| (1,1997) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HE1  | 7        | 0.59          |
| (1,1997) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HE1  | 7        | 0.59          |
| (1,1997) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HE1  | 7        | 0.59          |
| (1,1997) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HE1  | 7        | 0.59          |
| (1,1997) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HE1  | 7        | 0.59          |
| (1,1997) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HE1  | 7        | 0.59          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD11 | 6        | 0.57          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD12 | 6        | 0.57          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD13 | 6        | 0.57          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD21 | 6        | 0.57          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD22 | 6        | 0.57          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD23 | 6        | 0.57          |
| (1,1999) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HZ2  | 14       | 0.56          |
| (1,1999) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HZ2  | 14       | 0.56          |
| (1,1999) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HZ2  | 14       | 0.56          |
| (1,1999) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HZ2  | 14       | 0.56          |
| (1,1999) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HZ2  | 14       | 0.56          |
| (1,1999) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HZ2  | 14       | 0.56          |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG11 | 4        | 0.54          |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG12 | 4        | 0.54          |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG13 | 4        | 0.54          |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG21 | 4        | 0.54          |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG22 | 4        | 0.54          |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG23 | 4        | 0.54          |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG11 | 4        | 0.54          |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG12 | 4        | 0.54          |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG13 | 4        | 0.54          |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG21 | 4        | 0.54          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG22 | 4        | 0.54          |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG23 | 4        | 0.54          |
| (1,3425) | 1:488:A:LEU:HD11 | 1:489:A:TRP:HE1  | 7        | 0.52          |
| (1,3425) | 1:488:A:LEU:HD12 | 1:489:A:TRP:HE1  | 7        | 0.52          |
| (1,3425) | 1:488:A:LEU:HD13 | 1:489:A:TRP:HE1  | 7        | 0.52          |
| (1,3425) | 1:488:A:LEU:HD21 | 1:489:A:TRP:HE1  | 7        | 0.52          |
| (1,3425) | 1:488:A:LEU:HD22 | 1:489:A:TRP:HE1  | 7        | 0.52          |
| (1,3425) | 1:488:A:LEU:HD23 | 1:489:A:TRP:HE1  | 7        | 0.52          |
| (1,864)  | 1:303:A:ALA:HA   | 1:330:A:LEU:HD11 | 6        | 0.52          |
| (1,864)  | 1:303:A:ALA:HA   | 1:330:A:LEU:HD12 | 6        | 0.52          |
| (1,864)  | 1:303:A:ALA:HA   | 1:330:A:LEU:HD13 | 6        | 0.52          |
| (1,864)  | 1:303:A:ALA:HA   | 1:330:A:LEU:HD21 | 6        | 0.52          |
| (1,864)  | 1:303:A:ALA:HA   | 1:330:A:LEU:HD22 | 6        | 0.52          |
| (1,864)  | 1:303:A:ALA:HA   | 1:330:A:LEU:HD23 | 6        | 0.52          |
| (1,3425) | 1:488:A:LEU:HD11 | 1:489:A:TRP:HE1  | 13       | 0.51          |
| (1,3425) | 1:488:A:LEU:HD12 | 1:489:A:TRP:HE1  | 13       | 0.51          |
| (1,3425) | 1:488:A:LEU:HD13 | 1:489:A:TRP:HE1  | 13       | 0.51          |
| (1,3425) | 1:488:A:LEU:HD21 | 1:489:A:TRP:HE1  | 13       | 0.51          |
| (1,3425) | 1:488:A:LEU:HD22 | 1:489:A:TRP:HE1  | 13       | 0.51          |
| (1,3425) | 1:488:A:LEU:HD23 | 1:489:A:TRP:HE1  | 13       | 0.51          |
| (1,1221) | 1:330:A:LEU:HD11 | 1:350:A:SER:HA   | 10       | 0.5           |
| (1,1221) | 1:330:A:LEU:HD12 | 1:350:A:SER:HA   | 10       | 0.5           |
| (1,1221) | 1:330:A:LEU:HD13 | 1:350:A:SER:HA   | 10       | 0.5           |
| (1,1221) | 1:330:A:LEU:HD21 | 1:350:A:SER:HA   | 10       | 0.5           |
| (1,1221) | 1:330:A:LEU:HD22 | 1:350:A:SER:HA   | 10       | 0.5           |
| (1,1221) | 1:330:A:LEU:HD23 | 1:350:A:SER:HA   | 10       | 0.5           |
| (1,1223) | 1:330:A:LEU:HD11 | 1:351:A:GLY:H    | 1        | 0.48          |
| (1,1223) | 1:330:A:LEU:HD12 | 1:351:A:GLY:H    | 1        | 0.48          |
| (1,1223) | 1:330:A:LEU:HD13 | 1:351:A:GLY:H    | 1        | 0.48          |
| (1,1223) | 1:330:A:LEU:HD21 | 1:351:A:GLY:H    | 1        | 0.48          |
| (1,1223) | 1:330:A:LEU:HD22 | 1:351:A:GLY:H    | 1        | 0.48          |
| (1,1223) | 1:330:A:LEU:HD23 | 1:351:A:GLY:H    | 1        | 0.48          |
| (1,305)  | 1:265:A:TYR:HE1  | 1:272:A:LEU:HD11 | 4        | 0.48          |
| (1,305)  | 1:265:A:TYR:HE1  | 1:272:A:LEU:HD12 | 4        | 0.48          |
| (1,305)  | 1:265:A:TYR:HE1  | 1:272:A:LEU:HD13 | 4        | 0.48          |
| (1,305)  | 1:265:A:TYR:HE1  | 1:272:A:LEU:HD21 | 4        | 0.48          |
| (1,305)  | 1:265:A:TYR:HE1  | 1:272:A:LEU:HD22 | 4        | 0.48          |
| (1,305)  | 1:265:A:TYR:HE1  | 1:272:A:LEU:HD23 | 4        | 0.48          |
| (1,305)  | 1:265:A:TYR:HE2  | 1:272:A:LEU:HD11 | 4        | 0.48          |
| (1,305)  | 1:265:A:TYR:HE2  | 1:272:A:LEU:HD12 | 4        | 0.48          |
| (1,305)  | 1:265:A:TYR:HE2  | 1:272:A:LEU:HD13 | 4        | 0.48          |
| (1,305)  | 1:265:A:TYR:HE2  | 1:272:A:LEU:HD21 | 4        | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,305)  | 1:265:A:TYR:HE2  | 1:272:A:LEU:HD22 | 4        | 0.48          |
| (1,305)  | 1:265:A:TYR:HE2  | 1:272:A:LEU:HD23 | 4        | 0.48          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD11 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD12 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD13 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD21 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD22 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD23 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD11 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD12 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD13 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD21 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD22 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD23 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD11 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD12 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD13 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD21 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD22 | 15       | 0.45          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD23 | 15       | 0.45          |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG11 | 4        | 0.45          |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG12 | 4        | 0.45          |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG13 | 4        | 0.45          |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG21 | 4        | 0.45          |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG22 | 4        | 0.45          |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG23 | 4        | 0.45          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD11 | 3        | 0.44          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD12 | 3        | 0.44          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD13 | 3        | 0.44          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD21 | 3        | 0.44          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD22 | 3        | 0.44          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD23 | 3        | 0.44          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD11 | 3        | 0.44          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD12 | 3        | 0.44          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD13 | 3        | 0.44          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD21 | 3        | 0.44          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD22 | 3        | 0.44          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD23 | 3        | 0.44          |
| (1,3413) | 1:487:A:VAL:HG11 | 1:489:A:TRP:HD1  | 7        | 0.42          |
| (1,3413) | 1:487:A:VAL:HG12 | 1:489:A:TRP:HD1  | 7        | 0.42          |
| (1,3413) | 1:487:A:VAL:HG13 | 1:489:A:TRP:HD1  | 7        | 0.42          |
| (1,3413) | 1:487:A:VAL:HG21 | 1:489:A:TRP:HD1  | 7        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3413) | 1:487:A:VAL:HG22 | 1:489:A:TRP:HD1  | 7        | 0.42          |
| (1,3413) | 1:487:A:VAL:HG23 | 1:489:A:TRP:HD1  | 7        | 0.42          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG11 | 5        | 0.42          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG12 | 5        | 0.42          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG13 | 5        | 0.42          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG21 | 5        | 0.42          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG22 | 5        | 0.42          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG23 | 5        | 0.42          |
| (1,1223) | 1:330:A:LEU:HD11 | 1:351:A:GLY:H    | 7        | 0.41          |
| (1,1223) | 1:330:A:LEU:HD12 | 1:351:A:GLY:H    | 7        | 0.41          |
| (1,1223) | 1:330:A:LEU:HD13 | 1:351:A:GLY:H    | 7        | 0.41          |
| (1,1223) | 1:330:A:LEU:HD21 | 1:351:A:GLY:H    | 7        | 0.41          |
| (1,1223) | 1:330:A:LEU:HD22 | 1:351:A:GLY:H    | 7        | 0.41          |
| (1,1223) | 1:330:A:LEU:HD23 | 1:351:A:GLY:H    | 7        | 0.41          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG11 | 2        | 0.4           |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG12 | 2        | 0.4           |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG13 | 2        | 0.4           |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG21 | 2        | 0.4           |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG22 | 2        | 0.4           |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG23 | 2        | 0.4           |
| (1,3425) | 1:488:A:LEU:HD11 | 1:489:A:TRP:HE1  | 12       | 0.39          |
| (1,3425) | 1:488:A:LEU:HD12 | 1:489:A:TRP:HE1  | 12       | 0.39          |
| (1,3425) | 1:488:A:LEU:HD13 | 1:489:A:TRP:HE1  | 12       | 0.39          |
| (1,3425) | 1:488:A:LEU:HD21 | 1:489:A:TRP:HE1  | 12       | 0.39          |
| (1,3425) | 1:488:A:LEU:HD22 | 1:489:A:TRP:HE1  | 12       | 0.39          |
| (1,3425) | 1:488:A:LEU:HD23 | 1:489:A:TRP:HE1  | 12       | 0.39          |
| (1,1360) | 1:340:A:TYR:H    | 1:341:A:VAL:HG11 | 10       | 0.39          |
| (1,1360) | 1:340:A:TYR:H    | 1:341:A:VAL:HG12 | 10       | 0.39          |
| (1,1360) | 1:340:A:TYR:H    | 1:341:A:VAL:HG13 | 10       | 0.39          |
| (1,1360) | 1:340:A:TYR:H    | 1:341:A:VAL:HG21 | 10       | 0.39          |
| (1,1360) | 1:340:A:TYR:H    | 1:341:A:VAL:HG22 | 10       | 0.39          |
| (1,1360) | 1:340:A:TYR:H    | 1:341:A:VAL:HG23 | 10       | 0.39          |
| (1,3412) | 1:487:A:VAL:HG11 | 1:489:A:TRP:H    | 12       | 0.38          |
| (1,3412) | 1:487:A:VAL:HG12 | 1:489:A:TRP:H    | 12       | 0.38          |
| (1,3412) | 1:487:A:VAL:HG13 | 1:489:A:TRP:H    | 12       | 0.38          |
| (1,3412) | 1:487:A:VAL:HG21 | 1:489:A:TRP:H    | 12       | 0.38          |
| (1,3412) | 1:487:A:VAL:HG22 | 1:489:A:TRP:H    | 12       | 0.38          |
| (1,3412) | 1:487:A:VAL:HG23 | 1:489:A:TRP:H    | 12       | 0.38          |
| (1,1997) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HE1  | 8        | 0.38          |
| (1,1997) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HE1  | 8        | 0.38          |
| (1,1997) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HE1  | 8        | 0.38          |
| (1,1997) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HE1  | 8        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1997) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HE1  | 8        | 0.38          |
| (1,1997) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HE1  | 8        | 0.38          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG11 | 3        | 0.38          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG12 | 3        | 0.38          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG13 | 3        | 0.38          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG21 | 3        | 0.38          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG22 | 3        | 0.38          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG23 | 3        | 0.38          |
| (1,3425) | 1:488:A:LEU:HD11 | 1:489:A:TRP:HE1  | 15       | 0.37          |
| (1,3425) | 1:488:A:LEU:HD12 | 1:489:A:TRP:HE1  | 15       | 0.37          |
| (1,3425) | 1:488:A:LEU:HD13 | 1:489:A:TRP:HE1  | 15       | 0.37          |
| (1,3425) | 1:488:A:LEU:HD21 | 1:489:A:TRP:HE1  | 15       | 0.37          |
| (1,3425) | 1:488:A:LEU:HD22 | 1:489:A:TRP:HE1  | 15       | 0.37          |
| (1,3425) | 1:488:A:LEU:HD23 | 1:489:A:TRP:HE1  | 15       | 0.37          |
| (1,3413) | 1:487:A:VAL:HG11 | 1:489:A:TRP:HD1  | 8        | 0.37          |
| (1,3413) | 1:487:A:VAL:HG12 | 1:489:A:TRP:HD1  | 8        | 0.37          |
| (1,3413) | 1:487:A:VAL:HG13 | 1:489:A:TRP:HD1  | 8        | 0.37          |
| (1,3413) | 1:487:A:VAL:HG21 | 1:489:A:TRP:HD1  | 8        | 0.37          |
| (1,3413) | 1:487:A:VAL:HG22 | 1:489:A:TRP:HD1  | 8        | 0.37          |
| (1,3413) | 1:487:A:VAL:HG23 | 1:489:A:TRP:HD1  | 8        | 0.37          |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG11 | 14       | 0.37          |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG12 | 14       | 0.37          |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG13 | 14       | 0.37          |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG21 | 14       | 0.37          |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG22 | 14       | 0.37          |
| (1,2052) | 1:412:A:LYS:HE2  | 1:452:A:VAL:HG23 | 14       | 0.37          |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG11 | 14       | 0.37          |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG12 | 14       | 0.37          |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG13 | 14       | 0.37          |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG21 | 14       | 0.37          |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG22 | 14       | 0.37          |
| (1,2052) | 1:412:A:LYS:HE3  | 1:452:A:VAL:HG23 | 14       | 0.37          |
| (1,996)  | 1:316:A:LEU:HD11 | 1:318:A:GLU:H    | 6        | 0.37          |
| (1,996)  | 1:316:A:LEU:HD12 | 1:318:A:GLU:H    | 6        | 0.37          |
| (1,996)  | 1:316:A:LEU:HD13 | 1:318:A:GLU:H    | 6        | 0.37          |
| (1,996)  | 1:316:A:LEU:HD21 | 1:318:A:GLU:H    | 6        | 0.37          |
| (1,996)  | 1:316:A:LEU:HD22 | 1:318:A:GLU:H    | 6        | 0.37          |
| (1,996)  | 1:316:A:LEU:HD23 | 1:318:A:GLU:H    | 6        | 0.37          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD11 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD12 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD13 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD21 | 12       | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD22 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD23 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD11 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD12 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD13 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD21 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD22 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD23 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD11 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD12 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD13 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD21 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD22 | 12       | 0.36          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD23 | 12       | 0.36          |
| (1,1215) | 1:330:A:LEU:HD11 | 1:333:A:TYR:HE1  | 8        | 0.35          |
| (1,1215) | 1:330:A:LEU:HD11 | 1:333:A:TYR:HE2  | 8        | 0.35          |
| (1,1215) | 1:330:A:LEU:HD12 | 1:333:A:TYR:HE1  | 8        | 0.35          |
| (1,1215) | 1:330:A:LEU:HD12 | 1:333:A:TYR:HE2  | 8        | 0.35          |
| (1,1215) | 1:330:A:LEU:HD13 | 1:333:A:TYR:HE1  | 8        | 0.35          |
| (1,1215) | 1:330:A:LEU:HD13 | 1:333:A:TYR:HE2  | 8        | 0.35          |
| (1,1215) | 1:330:A:LEU:HD21 | 1:333:A:TYR:HE1  | 8        | 0.35          |
| (1,1215) | 1:330:A:LEU:HD21 | 1:333:A:TYR:HE2  | 8        | 0.35          |
| (1,1215) | 1:330:A:LEU:HD22 | 1:333:A:TYR:HE1  | 8        | 0.35          |
| (1,1215) | 1:330:A:LEU:HD22 | 1:333:A:TYR:HE2  | 8        | 0.35          |
| (1,1215) | 1:330:A:LEU:HD23 | 1:333:A:TYR:HE1  | 8        | 0.35          |
| (1,1215) | 1:330:A:LEU:HD23 | 1:333:A:TYR:HE2  | 8        | 0.35          |
| (1,1209) | 1:330:A:LEU:HD11 | 1:331:A:SER:H    | 7        | 0.35          |
| (1,1209) | 1:330:A:LEU:HD12 | 1:331:A:SER:H    | 7        | 0.35          |
| (1,1209) | 1:330:A:LEU:HD13 | 1:331:A:SER:H    | 7        | 0.35          |
| (1,1209) | 1:330:A:LEU:HD21 | 1:331:A:SER:H    | 7        | 0.35          |
| (1,1209) | 1:330:A:LEU:HD22 | 1:331:A:SER:H    | 7        | 0.35          |
| (1,1209) | 1:330:A:LEU:HD23 | 1:331:A:SER:H    | 7        | 0.35          |
| (1,437)  | 1:282:A:VAL:HG11 | 1:379:A:MET:HA   | 11       | 0.35          |
| (1,437)  | 1:282:A:VAL:HG12 | 1:379:A:MET:HA   | 11       | 0.35          |
| (1,437)  | 1:282:A:VAL:HG13 | 1:379:A:MET:HA   | 11       | 0.35          |
| (1,437)  | 1:282:A:VAL:HG21 | 1:379:A:MET:HA   | 11       | 0.35          |
| (1,437)  | 1:282:A:VAL:HG22 | 1:379:A:MET:HA   | 11       | 0.35          |
| (1,437)  | 1:282:A:VAL:HG23 | 1:379:A:MET:HA   | 11       | 0.35          |
| (1,367)  | 1:270:A:TYR:HE1  | 1:272:A:LEU:HD11 | 3        | 0.35          |
| (1,367)  | 1:270:A:TYR:HE1  | 1:272:A:LEU:HD12 | 3        | 0.35          |
| (1,367)  | 1:270:A:TYR:HE1  | 1:272:A:LEU:HD13 | 3        | 0.35          |
| (1,367)  | 1:270:A:TYR:HE1  | 1:272:A:LEU:HD21 | 3        | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,367)  | 1:270:A:TYR:HE1  | 1:272:A:LEU:HD22 | 3        | 0.35          |
| (1,367)  | 1:270:A:TYR:HE1  | 1:272:A:LEU:HD23 | 3        | 0.35          |
| (1,367)  | 1:270:A:TYR:HE2  | 1:272:A:LEU:HD11 | 3        | 0.35          |
| (1,367)  | 1:270:A:TYR:HE2  | 1:272:A:LEU:HD12 | 3        | 0.35          |
| (1,367)  | 1:270:A:TYR:HE2  | 1:272:A:LEU:HD13 | 3        | 0.35          |
| (1,367)  | 1:270:A:TYR:HE2  | 1:272:A:LEU:HD21 | 3        | 0.35          |
| (1,367)  | 1:270:A:TYR:HE2  | 1:272:A:LEU:HD22 | 3        | 0.35          |
| (1,367)  | 1:270:A:TYR:HE2  | 1:272:A:LEU:HD23 | 3        | 0.35          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG11 | 1        | 0.34          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG12 | 1        | 0.34          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG13 | 1        | 0.34          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG21 | 1        | 0.34          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG22 | 1        | 0.34          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG23 | 1        | 0.34          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG11 | 1        | 0.34          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG12 | 1        | 0.34          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG13 | 1        | 0.34          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG21 | 1        | 0.34          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG22 | 1        | 0.34          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG23 | 1        | 0.34          |
| (1,1221) | 1:330:A:LEU:HD11 | 1:350:A:SER:HA   | 7        | 0.34          |
| (1,1221) | 1:330:A:LEU:HD12 | 1:350:A:SER:HA   | 7        | 0.34          |
| (1,1221) | 1:330:A:LEU:HD13 | 1:350:A:SER:HA   | 7        | 0.34          |
| (1,1221) | 1:330:A:LEU:HD21 | 1:350:A:SER:HA   | 7        | 0.34          |
| (1,1221) | 1:330:A:LEU:HD22 | 1:350:A:SER:HA   | 7        | 0.34          |
| (1,1221) | 1:330:A:LEU:HD23 | 1:350:A:SER:HA   | 7        | 0.34          |
| (4,14)   | 1:350:A:SER:N    | 1:290:A:THR:O    | 2        | 0.33          |
| (4,14)   | 1:350:A:SER:N    | 1:290:A:THR:O    | 8        | 0.33          |
| (1,1999) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HZ2  | 4        | 0.33          |
| (1,1999) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HZ2  | 4        | 0.33          |
| (1,1999) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HZ2  | 4        | 0.33          |
| (1,1999) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HZ2  | 4        | 0.33          |
| (1,1999) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HZ2  | 4        | 0.33          |
| (1,1999) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HZ2  | 4        | 0.33          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG11 | 7        | 0.33          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG12 | 7        | 0.33          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG13 | 7        | 0.33          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG21 | 7        | 0.33          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG22 | 7        | 0.33          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG23 | 7        | 0.33          |
| (1,759)  | 1:299:A:LYS:HA   | 1:341:A:VAL:HG11 | 10       | 0.33          |
| (1,759)  | 1:299:A:LYS:HA   | 1:341:A:VAL:HG12 | 10       | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,759)  | 1:299:A:LYS:HA   | 1:341:A:VAL:HG13 | 10       | 0.33          |
| (1,759)  | 1:299:A:LYS:HA   | 1:341:A:VAL:HG21 | 10       | 0.33          |
| (1,759)  | 1:299:A:LYS:HA   | 1:341:A:VAL:HG22 | 10       | 0.33          |
| (1,759)  | 1:299:A:LYS:HA   | 1:341:A:VAL:HG23 | 10       | 0.33          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 1        | 0.32          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 5        | 0.32          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 7        | 0.32          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 13       | 0.32          |
| (4,14)   | 1:350:A:SER:N    | 1:290:A:THR:O    | 10       | 0.32          |
| (4,11)   | 1:299:A:LYS:N    | 1:317:A:ILE:O    | 4        | 0.32          |
| (4,9)    | 1:316:A:LEU:N    | 1:325:A:GLN:O    | 4        | 0.32          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG11 | 3        | 0.32          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG12 | 3        | 0.32          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG13 | 3        | 0.32          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG21 | 3        | 0.32          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG22 | 3        | 0.32          |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG23 | 3        | 0.32          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG11 | 3        | 0.32          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG12 | 3        | 0.32          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG13 | 3        | 0.32          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG21 | 3        | 0.32          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG22 | 3        | 0.32          |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG23 | 3        | 0.32          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD11 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD12 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD13 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD21 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD22 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD23 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD11 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD12 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD13 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD21 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD22 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD23 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD11 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD12 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD13 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD21 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD22 | 13       | 0.32          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD23 | 13       | 0.32          |
| (1,1221) | 1:330:A:LEU:HD11 | 1:350:A:SER:HA   | 1        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1221) | 1:330:A:LEU:HD12 | 1:350:A:SER:HA   | 1        | 0.32          |
| (1,1221) | 1:330:A:LEU:HD13 | 1:350:A:SER:HA   | 1        | 0.32          |
| (1,1221) | 1:330:A:LEU:HD21 | 1:350:A:SER:HA   | 1        | 0.32          |
| (1,1221) | 1:330:A:LEU:HD22 | 1:350:A:SER:HA   | 1        | 0.32          |
| (1,1221) | 1:330:A:LEU:HD23 | 1:350:A:SER:HA   | 1        | 0.32          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD11 | 14       | 0.32          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD12 | 14       | 0.32          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD13 | 14       | 0.32          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD21 | 14       | 0.32          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD22 | 14       | 0.32          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD23 | 14       | 0.32          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD11 | 14       | 0.32          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD12 | 14       | 0.32          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD13 | 14       | 0.32          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD21 | 14       | 0.32          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD22 | 14       | 0.32          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD23 | 14       | 0.32          |
| (1,437)  | 1:282:A:VAL:HG11 | 1:379:A:MET:HA   | 9        | 0.32          |
| (1,437)  | 1:282:A:VAL:HG12 | 1:379:A:MET:HA   | 9        | 0.32          |
| (1,437)  | 1:282:A:VAL:HG13 | 1:379:A:MET:HA   | 9        | 0.32          |
| (1,437)  | 1:282:A:VAL:HG21 | 1:379:A:MET:HA   | 9        | 0.32          |
| (1,437)  | 1:282:A:VAL:HG22 | 1:379:A:MET:HA   | 9        | 0.32          |
| (1,437)  | 1:282:A:VAL:HG23 | 1:379:A:MET:HA   | 9        | 0.32          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 2        | 0.31          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 3        | 0.31          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 4        | 0.31          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 10       | 0.31          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 14       | 0.31          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 15       | 0.31          |
| (4,14)   | 1:350:A:SER:N    | 1:290:A:THR:O    | 9        | 0.31          |
| (4,8)    | 1:314:A:ILE:O    | 1:327:A:TYR:N    | 2        | 0.31          |
| (4,8)    | 1:314:A:ILE:O    | 1:327:A:TYR:N    | 4        | 0.31          |
| (4,8)    | 1:314:A:ILE:O    | 1:327:A:TYR:N    | 9        | 0.31          |
| (4,8)    | 1:314:A:ILE:O    | 1:327:A:TYR:N    | 10       | 0.31          |
| (4,8)    | 1:314:A:ILE:O    | 1:327:A:TYR:N    | 14       | 0.31          |
| (4,3)    | 1:364:A:GLN:N    | 1:326:A:TRP:O    | 3        | 0.31          |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 1        | 0.31          |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 2        | 0.31          |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 4        | 0.31          |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 8        | 0.31          |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 9        | 0.31          |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 12       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 14       | 0.31          |
| (1,3400) | 1:485:A:LEU:HD11 | 1:486:A:GLY:H    | 1        | 0.31          |
| (1,3400) | 1:485:A:LEU:HD12 | 1:486:A:GLY:H    | 1        | 0.31          |
| (1,3400) | 1:485:A:LEU:HD13 | 1:486:A:GLY:H    | 1        | 0.31          |
| (1,3400) | 1:485:A:LEU:HD21 | 1:486:A:GLY:H    | 1        | 0.31          |
| (1,3400) | 1:485:A:LEU:HD22 | 1:486:A:GLY:H    | 1        | 0.31          |
| (1,3400) | 1:485:A:LEU:HD23 | 1:486:A:GLY:H    | 1        | 0.31          |
| (1,3238) | 1:475:A:VAL:HG11 | 1:476:A:ARG:HD2  | 1        | 0.31          |
| (1,3238) | 1:475:A:VAL:HG11 | 1:476:A:ARG:HD3  | 1        | 0.31          |
| (1,3238) | 1:475:A:VAL:HG12 | 1:476:A:ARG:HD2  | 1        | 0.31          |
| (1,3238) | 1:475:A:VAL:HG12 | 1:476:A:ARG:HD3  | 1        | 0.31          |
| (1,3238) | 1:475:A:VAL:HG13 | 1:476:A:ARG:HD2  | 1        | 0.31          |
| (1,3238) | 1:475:A:VAL:HG13 | 1:476:A:ARG:HD3  | 1        | 0.31          |
| (1,3238) | 1:475:A:VAL:HG21 | 1:476:A:ARG:HD2  | 1        | 0.31          |
| (1,3238) | 1:475:A:VAL:HG21 | 1:476:A:ARG:HD3  | 1        | 0.31          |
| (1,3238) | 1:475:A:VAL:HG22 | 1:476:A:ARG:HD2  | 1        | 0.31          |
| (1,3238) | 1:475:A:VAL:HG22 | 1:476:A:ARG:HD3  | 1        | 0.31          |
| (1,3238) | 1:475:A:VAL:HG23 | 1:476:A:ARG:HD2  | 1        | 0.31          |
| (1,3238) | 1:475:A:VAL:HG23 | 1:476:A:ARG:HD3  | 1        | 0.31          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG11 | 1        | 0.31          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG12 | 1        | 0.31          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG13 | 1        | 0.31          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG21 | 1        | 0.31          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG22 | 1        | 0.31          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG23 | 1        | 0.31          |
| (1,1999) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HZ2  | 2        | 0.31          |
| (1,1999) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HZ2  | 2        | 0.31          |
| (1,1999) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HZ2  | 2        | 0.31          |
| (1,1999) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HZ2  | 2        | 0.31          |
| (1,1999) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HZ2  | 2        | 0.31          |
| (1,1999) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HZ2  | 2        | 0.31          |
| (1,1999) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HZ2  | 11       | 0.31          |
| (1,1999) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HZ2  | 11       | 0.31          |
| (1,1999) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HZ2  | 11       | 0.31          |
| (1,1999) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HZ2  | 11       | 0.31          |
| (1,1999) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HZ2  | 11       | 0.31          |
| (1,1999) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HZ2  | 11       | 0.31          |
| (1,1999) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HZ2  | 15       | 0.31          |
| (1,1999) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HZ2  | 15       | 0.31          |
| (1,1999) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HZ2  | 15       | 0.31          |
| (1,1999) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HZ2  | 15       | 0.31          |
| (1,1999) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HZ2  | 15       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1999) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HZ2  | 15       | 0.31          |
| (1,1997) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HE1  | 5        | 0.31          |
| (1,1997) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HE1  | 5        | 0.31          |
| (1,1997) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HE1  | 5        | 0.31          |
| (1,1997) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HE1  | 5        | 0.31          |
| (1,1997) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HE1  | 5        | 0.31          |
| (1,1997) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HE1  | 5        | 0.31          |
| (4,14)   | 1:350:A:SER:N    | 1:290:A:THR:O    | 4        | 0.3           |
| (4,11)   | 1:299:A:LYS:N    | 1:317:A:ILE:O    | 14       | 0.3           |
| (4,9)    | 1:316:A:LEU:N    | 1:325:A:GLN:O    | 12       | 0.3           |
| (4,9)    | 1:316:A:LEU:N    | 1:325:A:GLN:O    | 14       | 0.3           |
| (4,8)    | 1:314:A:ILE:O    | 1:327:A:TYR:N    | 1        | 0.3           |
| (4,8)    | 1:314:A:ILE:O    | 1:327:A:TYR:N    | 13       | 0.3           |
| (4,3)    | 1:364:A:GLN:N    | 1:326:A:TRP:O    | 2        | 0.3           |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 3        | 0.3           |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 5        | 0.3           |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 6        | 0.3           |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 7        | 0.3           |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 10       | 0.3           |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 11       | 0.3           |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 15       | 0.3           |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG11 | 14       | 0.3           |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG12 | 14       | 0.3           |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG13 | 14       | 0.3           |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG21 | 14       | 0.3           |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG22 | 14       | 0.3           |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG23 | 14       | 0.3           |
| (1,1999) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HZ2  | 7        | 0.3           |
| (1,1999) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HZ2  | 7        | 0.3           |
| (1,1999) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HZ2  | 7        | 0.3           |
| (1,1999) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HZ2  | 7        | 0.3           |
| (1,1999) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HZ2  | 7        | 0.3           |
| (1,1999) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HZ2  | 7        | 0.3           |
| (1,1223) | 1:330:A:LEU:HD11 | 1:351:A:GLY:H    | 3        | 0.3           |
| (1,1223) | 1:330:A:LEU:HD12 | 1:351:A:GLY:H    | 3        | 0.3           |
| (1,1223) | 1:330:A:LEU:HD13 | 1:351:A:GLY:H    | 3        | 0.3           |
| (1,1223) | 1:330:A:LEU:HD21 | 1:351:A:GLY:H    | 3        | 0.3           |
| (1,1223) | 1:330:A:LEU:HD22 | 1:351:A:GLY:H    | 3        | 0.3           |
| (1,1223) | 1:330:A:LEU:HD23 | 1:351:A:GLY:H    | 3        | 0.3           |
| (1,1221) | 1:330:A:LEU:HD11 | 1:350:A:SER:HA   | 3        | 0.3           |
| (1,1221) | 1:330:A:LEU:HD12 | 1:350:A:SER:HA   | 3        | 0.3           |
| (1,1221) | 1:330:A:LEU:HD13 | 1:350:A:SER:HA   | 3        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1221) | 1:330:A:LEU:HD21 | 1:350:A:SER:HA   | 3        | 0.3           |
| (1,1221) | 1:330:A:LEU:HD22 | 1:350:A:SER:HA   | 3        | 0.3           |
| (1,1221) | 1:330:A:LEU:HD23 | 1:350:A:SER:HA   | 3        | 0.3           |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD11 | 4        | 0.3           |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD12 | 4        | 0.3           |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD13 | 4        | 0.3           |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD21 | 4        | 0.3           |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD22 | 4        | 0.3           |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD23 | 4        | 0.3           |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD11 | 4        | 0.3           |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD12 | 4        | 0.3           |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD13 | 4        | 0.3           |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD21 | 4        | 0.3           |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD22 | 4        | 0.3           |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD23 | 4        | 0.3           |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 6        | 0.29          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 8        | 0.29          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 11       | 0.29          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 12       | 0.29          |
| (4,14)   | 1:350:A:SER:N    | 1:290:A:THR:O    | 6        | 0.29          |
| (4,14)   | 1:350:A:SER:N    | 1:290:A:THR:O    | 15       | 0.29          |
| (4,9)    | 1:316:A:LEU:N    | 1:325:A:GLN:O    | 2        | 0.29          |
| (4,3)    | 1:364:A:GLN:N    | 1:326:A:TRP:O    | 1        | 0.29          |
| (4,3)    | 1:364:A:GLN:N    | 1:326:A:TRP:O    | 9        | 0.29          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG11 | 11       | 0.29          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG12 | 11       | 0.29          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG13 | 11       | 0.29          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG21 | 11       | 0.29          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG22 | 11       | 0.29          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG23 | 11       | 0.29          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG11 | 12       | 0.29          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG12 | 12       | 0.29          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG13 | 12       | 0.29          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG21 | 12       | 0.29          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG22 | 12       | 0.29          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG23 | 12       | 0.29          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD11 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD12 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD13 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD21 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD22 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD11 | 1:488:A:LEU:HD23 | 7        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD11 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD12 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD13 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD21 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD22 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD12 | 1:488:A:LEU:HD23 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD11 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD12 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD13 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD21 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD22 | 7        | 0.29          |
| (1,2365) | 1:424:A:ILE:HD13 | 1:488:A:LEU:HD23 | 7        | 0.29          |
| (1,1375) | 1:341:A:VAL:HG11 | 1:343:A:ALA:H    | 4        | 0.29          |
| (1,1375) | 1:341:A:VAL:HG12 | 1:343:A:ALA:H    | 4        | 0.29          |
| (1,1375) | 1:341:A:VAL:HG13 | 1:343:A:ALA:H    | 4        | 0.29          |
| (1,1375) | 1:341:A:VAL:HG21 | 1:343:A:ALA:H    | 4        | 0.29          |
| (1,1375) | 1:341:A:VAL:HG22 | 1:343:A:ALA:H    | 4        | 0.29          |
| (1,1375) | 1:341:A:VAL:HG23 | 1:343:A:ALA:H    | 4        | 0.29          |
| (4,14)   | 1:350:A:SER:N    | 1:290:A:THR:O    | 5        | 0.28          |
| (4,11)   | 1:299:A:LYS:N    | 1:317:A:ILE:O    | 2        | 0.28          |
| (4,11)   | 1:299:A:LYS:N    | 1:317:A:ILE:O    | 8        | 0.28          |
| (4,11)   | 1:299:A:LYS:N    | 1:317:A:ILE:O    | 13       | 0.28          |
| (4,9)    | 1:316:A:LEU:N    | 1:325:A:GLN:O    | 10       | 0.28          |
| (4,9)    | 1:316:A:LEU:N    | 1:325:A:GLN:O    | 11       | 0.28          |
| (4,9)    | 1:316:A:LEU:N    | 1:325:A:GLN:O    | 13       | 0.28          |
| (4,8)    | 1:314:A:ILE:O    | 1:327:A:TYR:N    | 3        | 0.28          |
| (4,8)    | 1:314:A:ILE:O    | 1:327:A:TYR:N    | 12       | 0.28          |
| (4,3)    | 1:364:A:GLN:N    | 1:326:A:TRP:O    | 5        | 0.28          |
| (4,3)    | 1:364:A:GLN:N    | 1:326:A:TRP:O    | 6        | 0.28          |
| (4,3)    | 1:364:A:GLN:N    | 1:326:A:TRP:O    | 10       | 0.28          |
| (4,3)    | 1:364:A:GLN:N    | 1:326:A:TRP:O    | 13       | 0.28          |
| (4,3)    | 1:364:A:GLN:N    | 1:326:A:TRP:O    | 15       | 0.28          |
| (4,2)    | 1:282:A:VAL:O    | 1:363:A:PHE:N    | 13       | 0.28          |
| (1,958)  | 1:314:A:ILE:HA   | 1:330:A:LEU:HD11 | 6        | 0.28          |
| (1,958)  | 1:314:A:ILE:HA   | 1:330:A:LEU:HD12 | 6        | 0.28          |
| (1,958)  | 1:314:A:ILE:HA   | 1:330:A:LEU:HD13 | 6        | 0.28          |
| (1,958)  | 1:314:A:ILE:HA   | 1:330:A:LEU:HD21 | 6        | 0.28          |
| (1,958)  | 1:314:A:ILE:HA   | 1:330:A:LEU:HD22 | 6        | 0.28          |
| (1,958)  | 1:314:A:ILE:HA   | 1:330:A:LEU:HD23 | 6        | 0.28          |
| (4,21)   | 1:471:A:ILE:N    | 1:463:A:TYR:O    | 12       | 0.27          |
| (4,20)   | 1:473:A:LEU:N    | 1:461:A:VAL:O    | 9        | 0.27          |
| (4,14)   | 1:350:A:SER:N    | 1:290:A:THR:O    | 3        | 0.27          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (4,11)   | 1:299:A:LYS:N   | 1:317:A:ILE:O    | 6        | 0.27          |
| (4,11)   | 1:299:A:LYS:N   | 1:317:A:ILE:O    | 12       | 0.27          |
| (4,8)    | 1:314:A:ILE:O   | 1:327:A:TYR:N    | 11       | 0.27          |
| (4,7)    | 1:314:A:ILE:N   | 1:327:A:TYR:O    | 4        | 0.27          |
| (4,5)    | 1:366:A:MET:N   | 1:324:A:ARG:O    | 1        | 0.27          |
| (4,3)    | 1:364:A:GLN:N   | 1:326:A:TRP:O    | 4        | 0.27          |
| (4,3)    | 1:364:A:GLN:N   | 1:326:A:TRP:O    | 12       | 0.27          |
| (4,3)    | 1:364:A:GLN:N   | 1:326:A:TRP:O    | 14       | 0.27          |
| (4,2)    | 1:282:A:VAL:O   | 1:363:A:PHE:N    | 11       | 0.27          |
| (4,1)    | 1:282:A:VAL:N   | 1:363:A:PHE:O    | 11       | 0.27          |
| (4,1)    | 1:282:A:VAL:N   | 1:363:A:PHE:O    | 12       | 0.27          |
| (1,2793) | 1:451:A:GLU:H   | 1:452:A:VAL:HG11 | 9        | 0.27          |
| (1,2793) | 1:451:A:GLU:H   | 1:452:A:VAL:HG12 | 9        | 0.27          |
| (1,2793) | 1:451:A:GLU:H   | 1:452:A:VAL:HG13 | 9        | 0.27          |
| (1,2793) | 1:451:A:GLU:H   | 1:452:A:VAL:HG21 | 9        | 0.27          |
| (1,2793) | 1:451:A:GLU:H   | 1:452:A:VAL:HG22 | 9        | 0.27          |
| (1,2793) | 1:451:A:GLU:H   | 1:452:A:VAL:HG23 | 9        | 0.27          |
| (1,2757) | 1:449:A:TYR:HD1 | 1:452:A:VAL:HG11 | 9        | 0.27          |
| (1,2757) | 1:449:A:TYR:HD1 | 1:452:A:VAL:HG12 | 9        | 0.27          |
| (1,2757) | 1:449:A:TYR:HD1 | 1:452:A:VAL:HG13 | 9        | 0.27          |
| (1,2757) | 1:449:A:TYR:HD1 | 1:452:A:VAL:HG21 | 9        | 0.27          |
| (1,2757) | 1:449:A:TYR:HD1 | 1:452:A:VAL:HG22 | 9        | 0.27          |
| (1,2757) | 1:449:A:TYR:HD1 | 1:452:A:VAL:HG23 | 9        | 0.27          |
| (1,2757) | 1:449:A:TYR:HD2 | 1:452:A:VAL:HG11 | 9        | 0.27          |
| (1,2757) | 1:449:A:TYR:HD2 | 1:452:A:VAL:HG12 | 9        | 0.27          |
| (1,2757) | 1:449:A:TYR:HD2 | 1:452:A:VAL:HG13 | 9        | 0.27          |
| (1,2757) | 1:449:A:TYR:HD2 | 1:452:A:VAL:HG21 | 9        | 0.27          |
| (1,2757) | 1:449:A:TYR:HD2 | 1:452:A:VAL:HG22 | 9        | 0.27          |
| (1,2757) | 1:449:A:TYR:HD2 | 1:452:A:VAL:HG23 | 9        | 0.27          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD11 | 11       | 0.27          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD12 | 11       | 0.27          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD13 | 11       | 0.27          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD21 | 11       | 0.27          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD22 | 11       | 0.27          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD23 | 11       | 0.27          |
| (1,1577) | 1:367:A:VAL:HB  | 1:369:A:SER:H    | 15       | 0.27          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD11 | 7        | 0.27          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD12 | 7        | 0.27          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD13 | 7        | 0.27          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD21 | 7        | 0.27          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD22 | 7        | 0.27          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD23 | 7        | 0.27          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD11 | 7        | 0.27          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD12 | 7        | 0.27          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD13 | 7        | 0.27          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD21 | 7        | 0.27          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD22 | 7        | 0.27          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD23 | 7        | 0.27          |
| (4,9)    | 1:316:A:LEU:N   | 1:325:A:GLN:O    | 6        | 0.26          |
| (4,9)    | 1:316:A:LEU:N   | 1:325:A:GLN:O    | 8        | 0.26          |
| (4,7)    | 1:314:A:ILE:N   | 1:327:A:TYR:O    | 12       | 0.26          |
| (4,6)    | 1:366:A:MET:O   | 1:324:A:ARG:N    | 13       | 0.26          |
| (4,4)    | 1:364:A:GLN:O   | 1:326:A:TRP:N    | 1        | 0.26          |
| (1,3283) | 1:477:A:THR:H   | 1:485:A:LEU:HD11 | 10       | 0.26          |
| (1,3283) | 1:477:A:THR:H   | 1:485:A:LEU:HD12 | 10       | 0.26          |
| (1,3283) | 1:477:A:THR:H   | 1:485:A:LEU:HD13 | 10       | 0.26          |
| (1,3283) | 1:477:A:THR:H   | 1:485:A:LEU:HD21 | 10       | 0.26          |
| (1,3283) | 1:477:A:THR:H   | 1:485:A:LEU:HD22 | 10       | 0.26          |
| (1,3283) | 1:477:A:THR:H   | 1:485:A:LEU:HD23 | 10       | 0.26          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD11 | 7        | 0.26          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD12 | 7        | 0.26          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD13 | 7        | 0.26          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD21 | 7        | 0.26          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD22 | 7        | 0.26          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD23 | 7        | 0.26          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD11 | 5        | 0.26          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD12 | 5        | 0.26          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD13 | 5        | 0.26          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD21 | 5        | 0.26          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD22 | 5        | 0.26          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD23 | 5        | 0.26          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD11 | 5        | 0.26          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD12 | 5        | 0.26          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD13 | 5        | 0.26          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD21 | 5        | 0.26          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD22 | 5        | 0.26          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD23 | 5        | 0.26          |
| (4,15)   | 1:383:A:LYS:N   | 1:380:A:PRO:O    | 12       | 0.25          |
| (4,11)   | 1:299:A:LYS:N   | 1:317:A:ILE:O    | 3        | 0.25          |
| (4,11)   | 1:299:A:LYS:N   | 1:317:A:ILE:O    | 10       | 0.25          |
| (4,9)    | 1:316:A:LEU:N   | 1:325:A:GLN:O    | 1        | 0.25          |
| (4,8)    | 1:314:A:ILE:O   | 1:327:A:TYR:N    | 5        | 0.25          |
| (4,8)    | 1:314:A:ILE:O   | 1:327:A:TYR:N    | 8        | 0.25          |
| (4,8)    | 1:314:A:ILE:O   | 1:327:A:TYR:N    | 15       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (4,6)    | 1:366:A:MET:O    | 1:324:A:ARG:N    | 4        | 0.25          |
| (4,3)    | 1:364:A:GLN:N    | 1:326:A:TRP:O    | 8        | 0.25          |
| (4,2)    | 1:282:A:VAL:O    | 1:363:A:PHE:N    | 7        | 0.25          |
| (4,1)    | 1:282:A:VAL:N    | 1:363:A:PHE:O    | 2        | 0.25          |
| (4,1)    | 1:282:A:VAL:N    | 1:363:A:PHE:O    | 8        | 0.25          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD11 | 1        | 0.25          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD12 | 1        | 0.25          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD13 | 1        | 0.25          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD21 | 1        | 0.25          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD22 | 1        | 0.25          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD23 | 1        | 0.25          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG11 | 6        | 0.25          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG12 | 6        | 0.25          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG13 | 6        | 0.25          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG21 | 6        | 0.25          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG22 | 6        | 0.25          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG23 | 6        | 0.25          |
| (1,2666) | 1:440:A:VAL:HG11 | 1:442:A:LYS:H    | 2        | 0.25          |
| (1,2666) | 1:440:A:VAL:HG12 | 1:442:A:LYS:H    | 2        | 0.25          |
| (1,2666) | 1:440:A:VAL:HG13 | 1:442:A:LYS:H    | 2        | 0.25          |
| (1,2666) | 1:440:A:VAL:HG21 | 1:442:A:LYS:H    | 2        | 0.25          |
| (1,2666) | 1:440:A:VAL:HG22 | 1:442:A:LYS:H    | 2        | 0.25          |
| (1,2666) | 1:440:A:VAL:HG23 | 1:442:A:LYS:H    | 2        | 0.25          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD11 | 7        | 0.25          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD12 | 7        | 0.25          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD13 | 7        | 0.25          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD21 | 7        | 0.25          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD22 | 7        | 0.25          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD23 | 7        | 0.25          |
| (1,1984) | 1:410:A:LEU:HD11 | 1:411:A:TYR:H    | 6        | 0.25          |
| (1,1984) | 1:410:A:LEU:HD12 | 1:411:A:TYR:H    | 6        | 0.25          |
| (1,1984) | 1:410:A:LEU:HD13 | 1:411:A:TYR:H    | 6        | 0.25          |
| (1,1984) | 1:410:A:LEU:HD21 | 1:411:A:TYR:H    | 6        | 0.25          |
| (1,1984) | 1:410:A:LEU:HD22 | 1:411:A:TYR:H    | 6        | 0.25          |
| (1,1984) | 1:410:A:LEU:HD23 | 1:411:A:TYR:H    | 6        | 0.25          |
| (1,1822) | 1:402:A:TRP:HZ2  | 1:452:A:VAL:HG11 | 3        | 0.25          |
| (1,1822) | 1:402:A:TRP:HZ2  | 1:452:A:VAL:HG12 | 3        | 0.25          |
| (1,1822) | 1:402:A:TRP:HZ2  | 1:452:A:VAL:HG13 | 3        | 0.25          |
| (1,1822) | 1:402:A:TRP:HZ2  | 1:452:A:VAL:HG21 | 3        | 0.25          |
| (1,1822) | 1:402:A:TRP:HZ2  | 1:452:A:VAL:HG22 | 3        | 0.25          |
| (1,1822) | 1:402:A:TRP:HZ2  | 1:452:A:VAL:HG23 | 3        | 0.25          |
| (1,1685) | 1:381:A:PHE:HZ   | 1:382:A:LEU:HD11 | 11       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1685) | 1:381:A:PHE:HZ   | 1:382:A:LEU:HD12 | 11       | 0.25          |
| (1,1685) | 1:381:A:PHE:HZ   | 1:382:A:LEU:HD13 | 11       | 0.25          |
| (1,1685) | 1:381:A:PHE:HZ   | 1:382:A:LEU:HD21 | 11       | 0.25          |
| (1,1685) | 1:381:A:PHE:HZ   | 1:382:A:LEU:HD22 | 11       | 0.25          |
| (1,1685) | 1:381:A:PHE:HZ   | 1:382:A:LEU:HD23 | 11       | 0.25          |
| (1,1577) | 1:367:A:VAL:HB   | 1:369:A:SER:H    | 8        | 0.25          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG11 | 6        | 0.25          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG12 | 6        | 0.25          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG13 | 6        | 0.25          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG21 | 6        | 0.25          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG22 | 6        | 0.25          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG23 | 6        | 0.25          |
| (4,12)   | 1:299:A:LYS:O    | 1:317:A:ILE:N    | 1        | 0.24          |
| (4,12)   | 1:299:A:LYS:O    | 1:317:A:ILE:N    | 4        | 0.24          |
| (4,9)    | 1:316:A:LEU:N    | 1:325:A:GLN:O    | 9        | 0.24          |
| (4,6)    | 1:366:A:MET:O    | 1:324:A:ARG:N    | 15       | 0.24          |
| (4,5)    | 1:366:A:MET:N    | 1:324:A:ARG:O    | 2        | 0.24          |
| (1,3467) | 1:492:A:ILE:HD11 | 1:493:A:LYS:H    | 11       | 0.24          |
| (1,3467) | 1:492:A:ILE:HD12 | 1:493:A:LYS:H    | 11       | 0.24          |
| (1,3467) | 1:492:A:ILE:HD13 | 1:493:A:LYS:H    | 11       | 0.24          |
| (1,2759) | 1:449:A:TYR:HE1  | 1:452:A:VAL:HG11 | 9        | 0.24          |
| (1,2759) | 1:449:A:TYR:HE1  | 1:452:A:VAL:HG12 | 9        | 0.24          |
| (1,2759) | 1:449:A:TYR:HE1  | 1:452:A:VAL:HG13 | 9        | 0.24          |
| (1,2759) | 1:449:A:TYR:HE1  | 1:452:A:VAL:HG21 | 9        | 0.24          |
| (1,2759) | 1:449:A:TYR:HE1  | 1:452:A:VAL:HG22 | 9        | 0.24          |
| (1,2759) | 1:449:A:TYR:HE1  | 1:452:A:VAL:HG23 | 9        | 0.24          |
| (1,2759) | 1:449:A:TYR:HE2  | 1:452:A:VAL:HG11 | 9        | 0.24          |
| (1,2759) | 1:449:A:TYR:HE2  | 1:452:A:VAL:HG12 | 9        | 0.24          |
| (1,2759) | 1:449:A:TYR:HE2  | 1:452:A:VAL:HG13 | 9        | 0.24          |
| (1,2759) | 1:449:A:TYR:HE2  | 1:452:A:VAL:HG21 | 9        | 0.24          |
| (1,2759) | 1:449:A:TYR:HE2  | 1:452:A:VAL:HG22 | 9        | 0.24          |
| (1,2759) | 1:449:A:TYR:HE2  | 1:452:A:VAL:HG23 | 9        | 0.24          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD11 | 5        | 0.24          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD12 | 5        | 0.24          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD13 | 5        | 0.24          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD21 | 5        | 0.24          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD22 | 5        | 0.24          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD23 | 5        | 0.24          |
| (4,21)   | 1:471:A:ILE:N    | 1:463:A:TYR:O    | 11       | 0.23          |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 14       | 0.23          |
| (4,11)   | 1:299:A:LYS:N    | 1:317:A:ILE:O    | 5        | 0.23          |
| (4,11)   | 1:299:A:LYS:N    | 1:317:A:ILE:O    | 9        | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (4,4)    | 1:364:A:GLN:O    | 1:326:A:TRP:N    | 13       | 0.23          |
| (4,2)    | 1:282:A:VAL:O    | 1:363:A:PHE:N    | 8        | 0.23          |
| (4,2)    | 1:282:A:VAL:O    | 1:363:A:PHE:N    | 14       | 0.23          |
| (4,1)    | 1:282:A:VAL:N    | 1:363:A:PHE:O    | 13       | 0.23          |
| (1,3412) | 1:487:A:VAL:HG11 | 1:489:A:TRP:H    | 7        | 0.23          |
| (1,3412) | 1:487:A:VAL:HG12 | 1:489:A:TRP:H    | 7        | 0.23          |
| (1,3412) | 1:487:A:VAL:HG13 | 1:489:A:TRP:H    | 7        | 0.23          |
| (1,3412) | 1:487:A:VAL:HG21 | 1:489:A:TRP:H    | 7        | 0.23          |
| (1,3412) | 1:487:A:VAL:HG22 | 1:489:A:TRP:H    | 7        | 0.23          |
| (1,3412) | 1:487:A:VAL:HG23 | 1:489:A:TRP:H    | 7        | 0.23          |
| (1,2666) | 1:440:A:VAL:HG11 | 1:442:A:LYS:H    | 12       | 0.23          |
| (1,2666) | 1:440:A:VAL:HG12 | 1:442:A:LYS:H    | 12       | 0.23          |
| (1,2666) | 1:440:A:VAL:HG13 | 1:442:A:LYS:H    | 12       | 0.23          |
| (1,2666) | 1:440:A:VAL:HG21 | 1:442:A:LYS:H    | 12       | 0.23          |
| (1,2666) | 1:440:A:VAL:HG22 | 1:442:A:LYS:H    | 12       | 0.23          |
| (1,2666) | 1:440:A:VAL:HG23 | 1:442:A:LYS:H    | 12       | 0.23          |
| (1,2050) | 1:412:A:LYS:H    | 1:452:A:VAL:HB   | 9        | 0.23          |
| (1,1577) | 1:367:A:VAL:HB   | 1:369:A:SER:H    | 6        | 0.23          |
| (1,1577) | 1:367:A:VAL:HB   | 1:369:A:SER:H    | 13       | 0.23          |
| (1,1375) | 1:341:A:VAL:HG11 | 1:343:A:ALA:H    | 2        | 0.23          |
| (1,1375) | 1:341:A:VAL:HG12 | 1:343:A:ALA:H    | 2        | 0.23          |
| (1,1375) | 1:341:A:VAL:HG13 | 1:343:A:ALA:H    | 2        | 0.23          |
| (1,1375) | 1:341:A:VAL:HG21 | 1:343:A:ALA:H    | 2        | 0.23          |
| (1,1375) | 1:341:A:VAL:HG22 | 1:343:A:ALA:H    | 2        | 0.23          |
| (1,1375) | 1:341:A:VAL:HG23 | 1:343:A:ALA:H    | 2        | 0.23          |
| (1,1223) | 1:330:A:LEU:HD11 | 1:351:A:GLY:H    | 11       | 0.23          |
| (1,1223) | 1:330:A:LEU:HD12 | 1:351:A:GLY:H    | 11       | 0.23          |
| (1,1223) | 1:330:A:LEU:HD13 | 1:351:A:GLY:H    | 11       | 0.23          |
| (1,1223) | 1:330:A:LEU:HD21 | 1:351:A:GLY:H    | 11       | 0.23          |
| (1,1223) | 1:330:A:LEU:HD22 | 1:351:A:GLY:H    | 11       | 0.23          |
| (1,1223) | 1:330:A:LEU:HD23 | 1:351:A:GLY:H    | 11       | 0.23          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG11 | 8        | 0.23          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG12 | 8        | 0.23          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG13 | 8        | 0.23          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG21 | 8        | 0.23          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG22 | 8        | 0.23          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG23 | 8        | 0.23          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG11 | 12       | 0.23          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG12 | 12       | 0.23          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG13 | 12       | 0.23          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG21 | 12       | 0.23          |
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG22 | 12       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,770)  | 1:300:A:ILE:HA   | 1:301:A:VAL:HG23 | 12       | 0.23          |
| (4,21)   | 1:471:A:ILE:N    | 1:463:A:TYR:O    | 14       | 0.22          |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 9        | 0.22          |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 10       | 0.22          |
| (4,15)   | 1:383:A:LYS:N    | 1:380:A:PRO:O    | 3        | 0.22          |
| (4,15)   | 1:383:A:LYS:N    | 1:380:A:PRO:O    | 8        | 0.22          |
| (4,4)    | 1:364:A:GLN:O    | 1:326:A:TRP:N    | 14       | 0.22          |
| (4,2)    | 1:282:A:VAL:O    | 1:363:A:PHE:N    | 1        | 0.22          |
| (4,2)    | 1:282:A:VAL:O    | 1:363:A:PHE:N    | 3        | 0.22          |
| (4,2)    | 1:282:A:VAL:O    | 1:363:A:PHE:N    | 9        | 0.22          |
| (4,2)    | 1:282:A:VAL:O    | 1:363:A:PHE:N    | 12       | 0.22          |
| (4,2)    | 1:282:A:VAL:O    | 1:363:A:PHE:N    | 15       | 0.22          |
| (4,1)    | 1:282:A:VAL:N    | 1:363:A:PHE:O    | 1        | 0.22          |
| (4,1)    | 1:282:A:VAL:N    | 1:363:A:PHE:O    | 10       | 0.22          |
| (1,3467) | 1:492:A:ILE:HD11 | 1:493:A:LYS:H    | 13       | 0.22          |
| (1,3467) | 1:492:A:ILE:HD12 | 1:493:A:LYS:H    | 13       | 0.22          |
| (1,3467) | 1:492:A:ILE:HD13 | 1:493:A:LYS:H    | 13       | 0.22          |
| (1,2823) | 1:452:A:VAL:HG11 | 1:462:A:GLY:H    | 9        | 0.22          |
| (1,2823) | 1:452:A:VAL:HG12 | 1:462:A:GLY:H    | 9        | 0.22          |
| (1,2823) | 1:452:A:VAL:HG13 | 1:462:A:GLY:H    | 9        | 0.22          |
| (1,2823) | 1:452:A:VAL:HG21 | 1:462:A:GLY:H    | 9        | 0.22          |
| (1,2823) | 1:452:A:VAL:HG22 | 1:462:A:GLY:H    | 9        | 0.22          |
| (1,2823) | 1:452:A:VAL:HG23 | 1:462:A:GLY:H    | 9        | 0.22          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG11 | 10       | 0.22          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG12 | 10       | 0.22          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG13 | 10       | 0.22          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG21 | 10       | 0.22          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG22 | 10       | 0.22          |
| (1,2799) | 1:451:A:GLU:HA   | 1:461:A:VAL:HG23 | 10       | 0.22          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG11 | 10       | 0.22          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG12 | 10       | 0.22          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG13 | 10       | 0.22          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG21 | 10       | 0.22          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG22 | 10       | 0.22          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG23 | 10       | 0.22          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG11 | 15       | 0.22          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG12 | 15       | 0.22          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG13 | 15       | 0.22          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG21 | 15       | 0.22          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG22 | 15       | 0.22          |
| (1,2083) | 1:414:A:GLU:H    | 1:452:A:VAL:HG23 | 15       | 0.22          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD11 | 1        | 0.22          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD12 | 1        | 0.22          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD13 | 1        | 0.22          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD21 | 1        | 0.22          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD22 | 1        | 0.22          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD23 | 1        | 0.22          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD11 | 1        | 0.22          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD12 | 1        | 0.22          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD13 | 1        | 0.22          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD21 | 1        | 0.22          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD22 | 1        | 0.22          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD23 | 1        | 0.22          |
| (4,21)   | 1:471:A:ILE:N   | 1:463:A:TYR:O    | 3        | 0.21          |
| (4,21)   | 1:471:A:ILE:N   | 1:463:A:TYR:O    | 5        | 0.21          |
| (4,15)   | 1:383:A:LYS:N   | 1:380:A:PRO:O    | 5        | 0.21          |
| (4,15)   | 1:383:A:LYS:N   | 1:380:A:PRO:O    | 10       | 0.21          |
| (4,15)   | 1:383:A:LYS:N   | 1:380:A:PRO:O    | 11       | 0.21          |
| (4,14)   | 1:350:A:SER:N   | 1:290:A:THR:O    | 7        | 0.21          |
| (4,14)   | 1:350:A:SER:N   | 1:290:A:THR:O    | 12       | 0.21          |
| (4,14)   | 1:350:A:SER:N   | 1:290:A:THR:O    | 14       | 0.21          |
| (4,11)   | 1:299:A:LYS:N   | 1:317:A:ILE:O    | 1        | 0.21          |
| (4,9)    | 1:316:A:LEU:N   | 1:325:A:GLN:O    | 3        | 0.21          |
| (4,7)    | 1:314:A:ILE:N   | 1:327:A:TYR:O    | 1        | 0.21          |
| (4,7)    | 1:314:A:ILE:N   | 1:327:A:TYR:O    | 7        | 0.21          |
| (4,6)    | 1:366:A:MET:O   | 1:324:A:ARG:N    | 12       | 0.21          |
| (4,5)    | 1:366:A:MET:N   | 1:324:A:ARG:O    | 6        | 0.21          |
| (4,3)    | 1:364:A:GLN:N   | 1:326:A:TRP:O    | 7        | 0.21          |
| (4,1)    | 1:282:A:VAL:N   | 1:363:A:PHE:O    | 3        | 0.21          |
| (4,1)    | 1:282:A:VAL:N   | 1:363:A:PHE:O    | 4        | 0.21          |
| (4,1)    | 1:282:A:VAL:N   | 1:363:A:PHE:O    | 7        | 0.21          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG11 | 4        | 0.21          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG12 | 4        | 0.21          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG13 | 4        | 0.21          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG21 | 4        | 0.21          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG22 | 4        | 0.21          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG23 | 4        | 0.21          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD11 | 10       | 0.21          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD12 | 10       | 0.21          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD13 | 10       | 0.21          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD21 | 10       | 0.21          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD22 | 10       | 0.21          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD23 | 10       | 0.21          |
| (1,1172) | 1:327:A:TYR:H   | 1:330:A:LEU:HD11 | 15       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD12 | 15       | 0.21          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD13 | 15       | 0.21          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD21 | 15       | 0.21          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD22 | 15       | 0.21          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD23 | 15       | 0.21          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD11 | 15       | 0.21          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD12 | 15       | 0.21          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD13 | 15       | 0.21          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD21 | 15       | 0.21          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD22 | 15       | 0.21          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD23 | 15       | 0.21          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD11 | 15       | 0.21          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD12 | 15       | 0.21          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD13 | 15       | 0.21          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD21 | 15       | 0.21          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD22 | 15       | 0.21          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD23 | 15       | 0.21          |
| (1,439)  | 1:282:A:VAL:HG11 | 1:379:A:MET:HG2  | 8        | 0.21          |
| (1,439)  | 1:282:A:VAL:HG11 | 1:379:A:MET:HG3  | 8        | 0.21          |
| (1,439)  | 1:282:A:VAL:HG12 | 1:379:A:MET:HG2  | 8        | 0.21          |
| (1,439)  | 1:282:A:VAL:HG12 | 1:379:A:MET:HG3  | 8        | 0.21          |
| (1,439)  | 1:282:A:VAL:HG13 | 1:379:A:MET:HG2  | 8        | 0.21          |
| (1,439)  | 1:282:A:VAL:HG13 | 1:379:A:MET:HG3  | 8        | 0.21          |
| (1,439)  | 1:282:A:VAL:HG21 | 1:379:A:MET:HG2  | 8        | 0.21          |
| (1,439)  | 1:282:A:VAL:HG21 | 1:379:A:MET:HG3  | 8        | 0.21          |
| (1,439)  | 1:282:A:VAL:HG22 | 1:379:A:MET:HG2  | 8        | 0.21          |
| (1,439)  | 1:282:A:VAL:HG22 | 1:379:A:MET:HG3  | 8        | 0.21          |
| (1,439)  | 1:282:A:VAL:HG23 | 1:379:A:MET:HG2  | 8        | 0.21          |
| (1,439)  | 1:282:A:VAL:HG23 | 1:379:A:MET:HG3  | 8        | 0.21          |
| (4,21)   | 1:471:A:ILE:N    | 1:463:A:TYR:O    | 4        | 0.2           |
| (4,21)   | 1:471:A:ILE:N    | 1:463:A:TYR:O    | 15       | 0.2           |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 7        | 0.2           |
| (4,15)   | 1:383:A:LYS:N    | 1:380:A:PRO:O    | 15       | 0.2           |
| (4,10)   | 1:316:A:LEU:O    | 1:325:A:GLN:N    | 1        | 0.2           |
| (4,9)    | 1:316:A:LEU:N    | 1:325:A:GLN:O    | 5        | 0.2           |
| (4,7)    | 1:314:A:ILE:N    | 1:327:A:TYR:O    | 9        | 0.2           |
| (4,6)    | 1:366:A:MET:O    | 1:324:A:ARG:N    | 8        | 0.2           |
| (4,6)    | 1:366:A:MET:O    | 1:324:A:ARG:N    | 11       | 0.2           |
| (4,5)    | 1:366:A:MET:N    | 1:324:A:ARG:O    | 9        | 0.2           |
| (4,4)    | 1:364:A:GLN:O    | 1:326:A:TRP:N    | 5        | 0.2           |
| (4,4)    | 1:364:A:GLN:O    | 1:326:A:TRP:N    | 8        | 0.2           |
| (4,3)    | 1:364:A:GLN:N    | 1:326:A:TRP:O    | 11       | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (4,1)    | 1:282:A:VAL:N    | 1:363:A:PHE:O    | 9        | 0.2           |
| (2,1)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 3        | 0.2           |
| (2,1)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 13       | 0.2           |
| (1,3467) | 1:492:A:ILE:HD11 | 1:493:A:LYS:H    | 10       | 0.2           |
| (1,3467) | 1:492:A:ILE:HD12 | 1:493:A:LYS:H    | 10       | 0.2           |
| (1,3467) | 1:492:A:ILE:HD13 | 1:493:A:LYS:H    | 10       | 0.2           |
| (1,3412) | 1:487:A:VAL:HG11 | 1:489:A:TRP:H    | 8        | 0.2           |
| (1,3412) | 1:487:A:VAL:HG12 | 1:489:A:TRP:H    | 8        | 0.2           |
| (1,3412) | 1:487:A:VAL:HG13 | 1:489:A:TRP:H    | 8        | 0.2           |
| (1,3412) | 1:487:A:VAL:HG21 | 1:489:A:TRP:H    | 8        | 0.2           |
| (1,3412) | 1:487:A:VAL:HG22 | 1:489:A:TRP:H    | 8        | 0.2           |
| (1,3412) | 1:487:A:VAL:HG23 | 1:489:A:TRP:H    | 8        | 0.2           |
| (1,3400) | 1:485:A:LEU:HD11 | 1:486:A:GLY:H    | 3        | 0.2           |
| (1,3400) | 1:485:A:LEU:HD12 | 1:486:A:GLY:H    | 3        | 0.2           |
| (1,3400) | 1:485:A:LEU:HD13 | 1:486:A:GLY:H    | 3        | 0.2           |
| (1,3400) | 1:485:A:LEU:HD21 | 1:486:A:GLY:H    | 3        | 0.2           |
| (1,3400) | 1:485:A:LEU:HD22 | 1:486:A:GLY:H    | 3        | 0.2           |
| (1,3400) | 1:485:A:LEU:HD23 | 1:486:A:GLY:H    | 3        | 0.2           |
| (1,2675) | 1:441:A:LEU:HD11 | 1:442:A:LYS:H    | 3        | 0.2           |
| (1,2675) | 1:441:A:LEU:HD12 | 1:442:A:LYS:H    | 3        | 0.2           |
| (1,2675) | 1:441:A:LEU:HD13 | 1:442:A:LYS:H    | 3        | 0.2           |
| (1,2675) | 1:441:A:LEU:HD21 | 1:442:A:LYS:H    | 3        | 0.2           |
| (1,2675) | 1:441:A:LEU:HD22 | 1:442:A:LYS:H    | 3        | 0.2           |
| (1,2675) | 1:441:A:LEU:HD23 | 1:442:A:LYS:H    | 3        | 0.2           |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG11 | 1        | 0.2           |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG12 | 1        | 0.2           |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG13 | 1        | 0.2           |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG21 | 1        | 0.2           |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG22 | 1        | 0.2           |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG23 | 1        | 0.2           |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG11 | 7        | 0.2           |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG12 | 7        | 0.2           |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG13 | 7        | 0.2           |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG21 | 7        | 0.2           |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG22 | 7        | 0.2           |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG23 | 7        | 0.2           |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG11 | 8        | 0.2           |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG12 | 8        | 0.2           |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG13 | 8        | 0.2           |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG21 | 8        | 0.2           |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG22 | 8        | 0.2           |
| (1,2644) | 1:437:A:GLN:HE21 | 1:440:A:VAL:HG23 | 8        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG11 | 8        | 0.2           |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG12 | 8        | 0.2           |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG13 | 8        | 0.2           |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG21 | 8        | 0.2           |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG22 | 8        | 0.2           |
| (1,2644) | 1:437:A:GLN:HE22 | 1:440:A:VAL:HG23 | 8        | 0.2           |
| (1,1221) | 1:330:A:LEU:HD11 | 1:350:A:SER:HA   | 14       | 0.2           |
| (1,1221) | 1:330:A:LEU:HD12 | 1:350:A:SER:HA   | 14       | 0.2           |
| (1,1221) | 1:330:A:LEU:HD13 | 1:350:A:SER:HA   | 14       | 0.2           |
| (1,1221) | 1:330:A:LEU:HD21 | 1:350:A:SER:HA   | 14       | 0.2           |
| (1,1221) | 1:330:A:LEU:HD22 | 1:350:A:SER:HA   | 14       | 0.2           |
| (1,1221) | 1:330:A:LEU:HD23 | 1:350:A:SER:HA   | 14       | 0.2           |
| (1,1082) | 1:322:A:VAL:HG11 | 1:324:A:ARG:H    | 6        | 0.2           |
| (1,1082) | 1:322:A:VAL:HG12 | 1:324:A:ARG:H    | 6        | 0.2           |
| (1,1082) | 1:322:A:VAL:HG13 | 1:324:A:ARG:H    | 6        | 0.2           |
| (1,1082) | 1:322:A:VAL:HG21 | 1:324:A:ARG:H    | 6        | 0.2           |
| (1,1082) | 1:322:A:VAL:HG22 | 1:324:A:ARG:H    | 6        | 0.2           |
| (1,1082) | 1:322:A:VAL:HG23 | 1:324:A:ARG:H    | 6        | 0.2           |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG11 | 9        | 0.2           |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG12 | 9        | 0.2           |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG13 | 9        | 0.2           |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG21 | 9        | 0.2           |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG22 | 9        | 0.2           |
| (1,1068) | 1:320:A:ASP:H    | 1:322:A:VAL:HG23 | 9        | 0.2           |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 3        | 0.19          |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 5        | 0.19          |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 11       | 0.19          |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 15       | 0.19          |
| (4,15)   | 1:383:A:LYS:N    | 1:380:A:PRO:O    | 7        | 0.19          |
| (4,14)   | 1:350:A:SER:N    | 1:290:A:THR:O    | 1        | 0.19          |
| (4,10)   | 1:316:A:LEU:O    | 1:325:A:GLN:N    | 14       | 0.19          |
| (4,9)    | 1:316:A:LEU:N    | 1:325:A:GLN:O    | 7        | 0.19          |
| (4,8)    | 1:314:A:ILE:O    | 1:327:A:TYR:N    | 7        | 0.19          |
| (4,7)    | 1:314:A:ILE:N    | 1:327:A:TYR:O    | 3        | 0.19          |
| (4,7)    | 1:314:A:ILE:N    | 1:327:A:TYR:O    | 8        | 0.19          |
| (4,6)    | 1:366:A:MET:O    | 1:324:A:ARG:N    | 6        | 0.19          |
| (4,5)    | 1:366:A:MET:N    | 1:324:A:ARG:O    | 7        | 0.19          |
| (4,4)    | 1:364:A:GLN:O    | 1:326:A:TRP:N    | 4        | 0.19          |
| (4,4)    | 1:364:A:GLN:O    | 1:326:A:TRP:N    | 6        | 0.19          |
| (4,4)    | 1:364:A:GLN:O    | 1:326:A:TRP:N    | 7        | 0.19          |
| (4,2)    | 1:282:A:VAL:O    | 1:363:A:PHE:N    | 4        | 0.19          |
| (4,2)    | 1:282:A:VAL:O    | 1:363:A:PHE:N    | 6        | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (4,1)    | 1:282:A:VAL:N    | 1:363:A:PHE:O    | 15       | 0.19          |
| (2,1)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 11       | 0.19          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG11 | 7        | 0.19          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG12 | 7        | 0.19          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG13 | 7        | 0.19          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG21 | 7        | 0.19          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG22 | 7        | 0.19          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG23 | 7        | 0.19          |
| (1,2666) | 1:440:A:VAL:HG11 | 1:442:A:LYS:H    | 11       | 0.19          |
| (1,2666) | 1:440:A:VAL:HG12 | 1:442:A:LYS:H    | 11       | 0.19          |
| (1,2666) | 1:440:A:VAL:HG13 | 1:442:A:LYS:H    | 11       | 0.19          |
| (1,2666) | 1:440:A:VAL:HG21 | 1:442:A:LYS:H    | 11       | 0.19          |
| (1,2666) | 1:440:A:VAL:HG22 | 1:442:A:LYS:H    | 11       | 0.19          |
| (1,2666) | 1:440:A:VAL:HG23 | 1:442:A:LYS:H    | 11       | 0.19          |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG11 | 3        | 0.19          |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG12 | 3        | 0.19          |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG13 | 3        | 0.19          |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG21 | 3        | 0.19          |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG22 | 3        | 0.19          |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG23 | 3        | 0.19          |
| (1,1209) | 1:330:A:LEU:HD11 | 1:331:A:SER:H    | 10       | 0.19          |
| (1,1209) | 1:330:A:LEU:HD12 | 1:331:A:SER:H    | 10       | 0.19          |
| (1,1209) | 1:330:A:LEU:HD13 | 1:331:A:SER:H    | 10       | 0.19          |
| (1,1209) | 1:330:A:LEU:HD21 | 1:331:A:SER:H    | 10       | 0.19          |
| (1,1209) | 1:330:A:LEU:HD22 | 1:331:A:SER:H    | 10       | 0.19          |
| (1,1209) | 1:330:A:LEU:HD23 | 1:331:A:SER:H    | 10       | 0.19          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG11 | 12       | 0.19          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG12 | 12       | 0.19          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG13 | 12       | 0.19          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG21 | 12       | 0.19          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG22 | 12       | 0.19          |
| (1,851)  | 1:302:A:GLU:HA   | 1:337:A:VAL:HG23 | 12       | 0.19          |
| (1,437)  | 1:282:A:VAL:HG11 | 1:379:A:MET:HA   | 15       | 0.19          |
| (1,437)  | 1:282:A:VAL:HG12 | 1:379:A:MET:HA   | 15       | 0.19          |
| (1,437)  | 1:282:A:VAL:HG13 | 1:379:A:MET:HA   | 15       | 0.19          |
| (1,437)  | 1:282:A:VAL:HG21 | 1:379:A:MET:HA   | 15       | 0.19          |
| (1,437)  | 1:282:A:VAL:HG22 | 1:379:A:MET:HA   | 15       | 0.19          |
| (1,437)  | 1:282:A:VAL:HG23 | 1:379:A:MET:HA   | 15       | 0.19          |
| (4,51)   | 1:383:A:LYS:H    | 1:380:A:PRO:O    | 2        | 0.18          |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 6        | 0.18          |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 8        | 0.18          |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 12       | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 13       | 0.18          |
| (4,15)   | 1:383:A:LYS:N    | 1:380:A:PRO:O    | 1        | 0.18          |
| (4,15)   | 1:383:A:LYS:N    | 1:380:A:PRO:O    | 2        | 0.18          |
| (4,13)   | 1:348:A:GLY:O    | 1:292:A:VAL:N    | 8        | 0.18          |
| (4,11)   | 1:299:A:LYS:N    | 1:317:A:ILE:O    | 15       | 0.18          |
| (4,6)    | 1:366:A:MET:O    | 1:324:A:ARG:N    | 9        | 0.18          |
| (4,4)    | 1:364:A:GLN:O    | 1:326:A:TRP:N    | 3        | 0.18          |
| (4,4)    | 1:364:A:GLN:O    | 1:326:A:TRP:N    | 10       | 0.18          |
| (4,1)    | 1:282:A:VAL:N    | 1:363:A:PHE:O    | 5        | 0.18          |
| (2,1)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 6        | 0.18          |
| (2,1)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 12       | 0.18          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD11 | 3        | 0.18          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD12 | 3        | 0.18          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD13 | 3        | 0.18          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD21 | 3        | 0.18          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD22 | 3        | 0.18          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD23 | 3        | 0.18          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD11 | 13       | 0.18          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD12 | 13       | 0.18          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD13 | 13       | 0.18          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD21 | 13       | 0.18          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD22 | 13       | 0.18          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD23 | 13       | 0.18          |
| (1,2253) | 1:420:A:PRO:HG3  | 1:441:A:LEU:HG   | 9        | 0.18          |
| (1,437)  | 1:282:A:VAL:HG11 | 1:379:A:MET:HA   | 10       | 0.18          |
| (1,437)  | 1:282:A:VAL:HG12 | 1:379:A:MET:HA   | 10       | 0.18          |
| (1,437)  | 1:282:A:VAL:HG13 | 1:379:A:MET:HA   | 10       | 0.18          |
| (1,437)  | 1:282:A:VAL:HG21 | 1:379:A:MET:HA   | 10       | 0.18          |
| (1,437)  | 1:282:A:VAL:HG22 | 1:379:A:MET:HA   | 10       | 0.18          |
| (1,437)  | 1:282:A:VAL:HG23 | 1:379:A:MET:HA   | 10       | 0.18          |
| (4,51)   | 1:383:A:LYS:H    | 1:380:A:PRO:O    | 7        | 0.17          |
| (4,51)   | 1:383:A:LYS:H    | 1:380:A:PRO:O    | 13       | 0.17          |
| (4,21)   | 1:471:A:ILE:N    | 1:463:A:TYR:O    | 13       | 0.17          |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 1        | 0.17          |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 2        | 0.17          |
| (4,15)   | 1:383:A:LYS:N    | 1:380:A:PRO:O    | 13       | 0.17          |
| (4,13)   | 1:348:A:GLY:O    | 1:292:A:VAL:N    | 9        | 0.17          |
| (4,12)   | 1:299:A:LYS:O    | 1:317:A:ILE:N    | 10       | 0.17          |
| (4,12)   | 1:299:A:LYS:O    | 1:317:A:ILE:N    | 14       | 0.17          |
| (4,11)   | 1:299:A:LYS:N    | 1:317:A:ILE:O    | 7        | 0.17          |
| (4,8)    | 1:314:A:ILE:O    | 1:327:A:TYR:N    | 6        | 0.17          |
| (4,7)    | 1:314:A:ILE:N    | 1:327:A:TYR:O    | 10       | 0.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (4,7)    | 1:314:A:ILE:N   | 1:327:A:TYR:O    | 14       | 0.17          |
| (4,6)    | 1:366:A:MET:O   | 1:324:A:ARG:N    | 1        | 0.17          |
| (4,5)    | 1:366:A:MET:N   | 1:324:A:ARG:O    | 3        | 0.17          |
| (4,5)    | 1:366:A:MET:N   | 1:324:A:ARG:O    | 11       | 0.17          |
| (4,4)    | 1:364:A:GLN:O   | 1:326:A:TRP:N    | 2        | 0.17          |
| (4,4)    | 1:364:A:GLN:O   | 1:326:A:TRP:N    | 12       | 0.17          |
| (4,2)    | 1:282:A:VAL:O   | 1:363:A:PHE:N    | 10       | 0.17          |
| (4,1)    | 1:282:A:VAL:N   | 1:363:A:PHE:O    | 6        | 0.17          |
| (1,3283) | 1:477:A:THR:H   | 1:485:A:LEU:HD11 | 4        | 0.17          |
| (1,3283) | 1:477:A:THR:H   | 1:485:A:LEU:HD12 | 4        | 0.17          |
| (1,3283) | 1:477:A:THR:H   | 1:485:A:LEU:HD13 | 4        | 0.17          |
| (1,3283) | 1:477:A:THR:H   | 1:485:A:LEU:HD21 | 4        | 0.17          |
| (1,3283) | 1:477:A:THR:H   | 1:485:A:LEU:HD22 | 4        | 0.17          |
| (1,3283) | 1:477:A:THR:H   | 1:485:A:LEU:HD23 | 4        | 0.17          |
| (1,2803) | 1:451:A:GLU:HB2 | 1:462:A:GLY:HA3  | 8        | 0.17          |
| (1,2803) | 1:451:A:GLU:HB3 | 1:462:A:GLY:HA3  | 8        | 0.17          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG11 | 2        | 0.17          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG12 | 2        | 0.17          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG13 | 2        | 0.17          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG21 | 2        | 0.17          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG22 | 2        | 0.17          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG23 | 2        | 0.17          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG11 | 7        | 0.17          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG12 | 7        | 0.17          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG13 | 7        | 0.17          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG21 | 7        | 0.17          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG22 | 7        | 0.17          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG23 | 7        | 0.17          |
| (1,2247) | 1:420:A:PRO:HB2 | 1:441:A:LEU:HD11 | 8        | 0.17          |
| (1,2247) | 1:420:A:PRO:HB2 | 1:441:A:LEU:HD12 | 8        | 0.17          |
| (1,2247) | 1:420:A:PRO:HB2 | 1:441:A:LEU:HD13 | 8        | 0.17          |
| (1,2247) | 1:420:A:PRO:HB2 | 1:441:A:LEU:HD21 | 8        | 0.17          |
| (1,2247) | 1:420:A:PRO:HB2 | 1:441:A:LEU:HD22 | 8        | 0.17          |
| (1,2247) | 1:420:A:PRO:HB2 | 1:441:A:LEU:HD23 | 8        | 0.17          |
| (1,2247) | 1:420:A:PRO:HB2 | 1:441:A:LEU:HD11 | 13       | 0.17          |
| (1,2247) | 1:420:A:PRO:HB2 | 1:441:A:LEU:HD12 | 13       | 0.17          |
| (1,2247) | 1:420:A:PRO:HB2 | 1:441:A:LEU:HD13 | 13       | 0.17          |
| (1,2247) | 1:420:A:PRO:HB2 | 1:441:A:LEU:HD21 | 13       | 0.17          |
| (1,2247) | 1:420:A:PRO:HB2 | 1:441:A:LEU:HD22 | 13       | 0.17          |
| (1,2247) | 1:420:A:PRO:HB2 | 1:441:A:LEU:HD23 | 13       | 0.17          |
| (1,2087) | 1:415:A:SER:HB2 | 1:416:A:ALA:H    | 11       | 0.17          |
| (1,2087) | 1:415:A:SER:HB3 | 1:416:A:ALA:H    | 11       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,996)  | 1:316:A:LEU:HD11 | 1:318:A:GLU:H    | 8        | 0.17          |
| (1,996)  | 1:316:A:LEU:HD12 | 1:318:A:GLU:H    | 8        | 0.17          |
| (1,996)  | 1:316:A:LEU:HD13 | 1:318:A:GLU:H    | 8        | 0.17          |
| (1,996)  | 1:316:A:LEU:HD21 | 1:318:A:GLU:H    | 8        | 0.17          |
| (1,996)  | 1:316:A:LEU:HD22 | 1:318:A:GLU:H    | 8        | 0.17          |
| (1,996)  | 1:316:A:LEU:HD23 | 1:318:A:GLU:H    | 8        | 0.17          |
| (1,872)  | 1:304:A:GLY:H    | 1:314:A:ILE:HB   | 13       | 0.17          |
| (1,437)  | 1:282:A:VAL:HG11 | 1:379:A:MET:HA   | 3        | 0.17          |
| (1,437)  | 1:282:A:VAL:HG12 | 1:379:A:MET:HA   | 3        | 0.17          |
| (1,437)  | 1:282:A:VAL:HG13 | 1:379:A:MET:HA   | 3        | 0.17          |
| (1,437)  | 1:282:A:VAL:HG21 | 1:379:A:MET:HA   | 3        | 0.17          |
| (1,437)  | 1:282:A:VAL:HG22 | 1:379:A:MET:HA   | 3        | 0.17          |
| (1,437)  | 1:282:A:VAL:HG23 | 1:379:A:MET:HA   | 3        | 0.17          |
| (4,15)   | 1:383:A:LYS:N    | 1:380:A:PRO:O    | 14       | 0.16          |
| (4,13)   | 1:348:A:GLY:O    | 1:292:A:VAL:N    | 4        | 0.16          |
| (4,12)   | 1:299:A:LYS:O    | 1:317:A:ILE:N    | 8        | 0.16          |
| (4,12)   | 1:299:A:LYS:O    | 1:317:A:ILE:N    | 15       | 0.16          |
| (4,11)   | 1:299:A:LYS:N    | 1:317:A:ILE:O    | 11       | 0.16          |
| (4,10)   | 1:316:A:LEU:O    | 1:325:A:GLN:N    | 11       | 0.16          |
| (4,9)    | 1:316:A:LEU:N    | 1:325:A:GLN:O    | 15       | 0.16          |
| (4,7)    | 1:314:A:ILE:N    | 1:327:A:TYR:O    | 2        | 0.16          |
| (4,7)    | 1:314:A:ILE:N    | 1:327:A:TYR:O    | 6        | 0.16          |
| (4,6)    | 1:366:A:MET:O    | 1:324:A:ARG:N    | 2        | 0.16          |
| (4,6)    | 1:366:A:MET:O    | 1:324:A:ARG:N    | 3        | 0.16          |
| (4,5)    | 1:366:A:MET:N    | 1:324:A:ARG:O    | 5        | 0.16          |
| (4,4)    | 1:364:A:GLN:O    | 1:326:A:TRP:N    | 11       | 0.16          |
| (4,2)    | 1:282:A:VAL:O    | 1:363:A:PHE:N    | 2        | 0.16          |
| (4,2)    | 1:282:A:VAL:O    | 1:363:A:PHE:N    | 5        | 0.16          |
| (4,1)    | 1:282:A:VAL:N    | 1:363:A:PHE:O    | 14       | 0.16          |
| (2,3)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 13       | 0.16          |
| (2,1)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 4        | 0.16          |
| (1,3471) | 1:492:A:ILE:HG21 | 1:493:A:LYS:HG2  | 3        | 0.16          |
| (1,3471) | 1:492:A:ILE:HG21 | 1:493:A:LYS:HG3  | 3        | 0.16          |
| (1,3471) | 1:492:A:ILE:HG22 | 1:493:A:LYS:HG2  | 3        | 0.16          |
| (1,3471) | 1:492:A:ILE:HG22 | 1:493:A:LYS:HG3  | 3        | 0.16          |
| (1,3471) | 1:492:A:ILE:HG23 | 1:493:A:LYS:HG2  | 3        | 0.16          |
| (1,3471) | 1:492:A:ILE:HG23 | 1:493:A:LYS:HG3  | 3        | 0.16          |
| (1,2803) | 1:451:A:GLU:HB2  | 1:462:A:GLY:HA3  | 6        | 0.16          |
| (1,2803) | 1:451:A:GLU:HB3  | 1:462:A:GLY:HA3  | 6        | 0.16          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD11 | 10       | 0.16          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD12 | 10       | 0.16          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD13 | 10       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD21 | 10       | 0.16          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD22 | 10       | 0.16          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD23 | 10       | 0.16          |
| (1,2087) | 1:415:A:SER:HB2  | 1:416:A:ALA:H    | 4        | 0.16          |
| (1,2087) | 1:415:A:SER:HB3  | 1:416:A:ALA:H    | 4        | 0.16          |
| (1,1378) | 1:341:A:VAL:HG11 | 1:345:A:GLN:H    | 4        | 0.16          |
| (1,1378) | 1:341:A:VAL:HG12 | 1:345:A:GLN:H    | 4        | 0.16          |
| (1,1378) | 1:341:A:VAL:HG13 | 1:345:A:GLN:H    | 4        | 0.16          |
| (1,1378) | 1:341:A:VAL:HG21 | 1:345:A:GLN:H    | 4        | 0.16          |
| (1,1378) | 1:341:A:VAL:HG22 | 1:345:A:GLN:H    | 4        | 0.16          |
| (1,1378) | 1:341:A:VAL:HG23 | 1:345:A:GLN:H    | 4        | 0.16          |
| (1,1375) | 1:341:A:VAL:HG11 | 1:343:A:ALA:H    | 13       | 0.16          |
| (1,1375) | 1:341:A:VAL:HG12 | 1:343:A:ALA:H    | 13       | 0.16          |
| (1,1375) | 1:341:A:VAL:HG13 | 1:343:A:ALA:H    | 13       | 0.16          |
| (1,1375) | 1:341:A:VAL:HG21 | 1:343:A:ALA:H    | 13       | 0.16          |
| (1,1375) | 1:341:A:VAL:HG22 | 1:343:A:ALA:H    | 13       | 0.16          |
| (1,1375) | 1:341:A:VAL:HG23 | 1:343:A:ALA:H    | 13       | 0.16          |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD11 | 9        | 0.16          |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD12 | 9        | 0.16          |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD13 | 9        | 0.16          |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD21 | 9        | 0.16          |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD22 | 9        | 0.16          |
| (1,957)  | 1:314:A:ILE:H    | 1:330:A:LEU:HD23 | 9        | 0.16          |
| (1,355)  | 1:268:A:GLY:H    | 1:269:A:PRO:HA   | 4        | 0.16          |
| (1,156)  | 1:257:A:TRP:HZ2  | 1:361:A:LEU:HD11 | 1        | 0.16          |
| (1,156)  | 1:257:A:TRP:HZ2  | 1:361:A:LEU:HD12 | 1        | 0.16          |
| (1,156)  | 1:257:A:TRP:HZ2  | 1:361:A:LEU:HD13 | 1        | 0.16          |
| (1,156)  | 1:257:A:TRP:HZ2  | 1:361:A:LEU:HD21 | 1        | 0.16          |
| (1,156)  | 1:257:A:TRP:HZ2  | 1:361:A:LEU:HD22 | 1        | 0.16          |
| (1,156)  | 1:257:A:TRP:HZ2  | 1:361:A:LEU:HD23 | 1        | 0.16          |
| (4,51)   | 1:383:A:LYS:H    | 1:380:A:PRO:O    | 9        | 0.15          |
| (4,51)   | 1:383:A:LYS:H    | 1:380:A:PRO:O    | 14       | 0.15          |
| (4,21)   | 1:471:A:ILE:N    | 1:463:A:TYR:O    | 7        | 0.15          |
| (4,21)   | 1:471:A:ILE:N    | 1:463:A:TYR:O    | 9        | 0.15          |
| (4,18)   | 1:424:A:ILE:N    | 1:441:A:LEU:O    | 4        | 0.15          |
| (4,15)   | 1:383:A:LYS:N    | 1:380:A:PRO:O    | 6        | 0.15          |
| (4,14)   | 1:350:A:SER:N    | 1:290:A:THR:O    | 13       | 0.15          |
| (4,13)   | 1:348:A:GLY:O    | 1:292:A:VAL:N    | 5        | 0.15          |
| (4,13)   | 1:348:A:GLY:O    | 1:292:A:VAL:N    | 6        | 0.15          |
| (4,12)   | 1:299:A:LYS:O    | 1:317:A:ILE:N    | 2        | 0.15          |
| (4,12)   | 1:299:A:LYS:O    | 1:317:A:ILE:N    | 6        | 0.15          |
| (4,12)   | 1:299:A:LYS:O    | 1:317:A:ILE:N    | 7        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (4,12)   | 1:299:A:LYS:O    | 1:317:A:ILE:N    | 9        | 0.15          |
| (4,12)   | 1:299:A:LYS:O    | 1:317:A:ILE:N    | 13       | 0.15          |
| (4,10)   | 1:316:A:LEU:O    | 1:325:A:GLN:N    | 2        | 0.15          |
| (4,10)   | 1:316:A:LEU:O    | 1:325:A:GLN:N    | 7        | 0.15          |
| (4,7)    | 1:314:A:ILE:N    | 1:327:A:TYR:O    | 5        | 0.15          |
| (4,7)    | 1:314:A:ILE:N    | 1:327:A:TYR:O    | 11       | 0.15          |
| (4,7)    | 1:314:A:ILE:N    | 1:327:A:TYR:O    | 15       | 0.15          |
| (4,6)    | 1:366:A:MET:O    | 1:324:A:ARG:N    | 10       | 0.15          |
| (2,1)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 1        | 0.15          |
| (1,3471) | 1:492:A:ILE:HG21 | 1:493:A:LYS:HG2  | 2        | 0.15          |
| (1,3471) | 1:492:A:ILE:HG21 | 1:493:A:LYS:HG3  | 2        | 0.15          |
| (1,3471) | 1:492:A:ILE:HG22 | 1:493:A:LYS:HG2  | 2        | 0.15          |
| (1,3471) | 1:492:A:ILE:HG22 | 1:493:A:LYS:HG3  | 2        | 0.15          |
| (1,3471) | 1:492:A:ILE:HG23 | 1:493:A:LYS:HG2  | 2        | 0.15          |
| (1,3471) | 1:492:A:ILE:HG23 | 1:493:A:LYS:HG3  | 2        | 0.15          |
| (1,3471) | 1:492:A:ILE:HG21 | 1:493:A:LYS:HG2  | 8        | 0.15          |
| (1,3471) | 1:492:A:ILE:HG21 | 1:493:A:LYS:HG3  | 8        | 0.15          |
| (1,3471) | 1:492:A:ILE:HG22 | 1:493:A:LYS:HG2  | 8        | 0.15          |
| (1,3471) | 1:492:A:ILE:HG22 | 1:493:A:LYS:HG3  | 8        | 0.15          |
| (1,3471) | 1:492:A:ILE:HG23 | 1:493:A:LYS:HG2  | 8        | 0.15          |
| (1,3471) | 1:492:A:ILE:HG23 | 1:493:A:LYS:HG3  | 8        | 0.15          |
| (1,3467) | 1:492:A:ILE:HD11 | 1:493:A:LYS:H    | 4        | 0.15          |
| (1,3467) | 1:492:A:ILE:HD12 | 1:493:A:LYS:H    | 4        | 0.15          |
| (1,3467) | 1:492:A:ILE:HD13 | 1:493:A:LYS:H    | 4        | 0.15          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD11 | 7        | 0.15          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD12 | 7        | 0.15          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD13 | 7        | 0.15          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD21 | 7        | 0.15          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD22 | 7        | 0.15          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD23 | 7        | 0.15          |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG11 | 8        | 0.15          |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG12 | 8        | 0.15          |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG13 | 8        | 0.15          |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG21 | 8        | 0.15          |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG22 | 8        | 0.15          |
| (1,2654) | 1:439:A:GLY:H    | 1:440:A:VAL:HG23 | 8        | 0.15          |
| (1,2603) | 1:433:A:ARG:HD2  | 1:434:A:SER:H    | 10       | 0.15          |
| (1,2603) | 1:433:A:ARG:HD3  | 1:434:A:SER:H    | 10       | 0.15          |
| (1,2087) | 1:415:A:SER:HB2  | 1:416:A:ALA:H    | 1        | 0.15          |
| (1,2087) | 1:415:A:SER:HB3  | 1:416:A:ALA:H    | 1        | 0.15          |
| (1,1683) | 1:381:A:PHE:HA   | 1:382:A:LEU:HD11 | 11       | 0.15          |
| (1,1683) | 1:381:A:PHE:HA   | 1:382:A:LEU:HD12 | 11       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1683) | 1:381:A:PHE:HA   | 1:382:A:LEU:HD13 | 11       | 0.15          |
| (1,1683) | 1:381:A:PHE:HA   | 1:382:A:LEU:HD21 | 11       | 0.15          |
| (1,1683) | 1:381:A:PHE:HA   | 1:382:A:LEU:HD22 | 11       | 0.15          |
| (1,1683) | 1:381:A:PHE:HA   | 1:382:A:LEU:HD23 | 11       | 0.15          |
| (1,1378) | 1:341:A:VAL:HG11 | 1:345:A:GLN:H    | 13       | 0.15          |
| (1,1378) | 1:341:A:VAL:HG12 | 1:345:A:GLN:H    | 13       | 0.15          |
| (1,1378) | 1:341:A:VAL:HG13 | 1:345:A:GLN:H    | 13       | 0.15          |
| (1,1378) | 1:341:A:VAL:HG21 | 1:345:A:GLN:H    | 13       | 0.15          |
| (1,1378) | 1:341:A:VAL:HG22 | 1:345:A:GLN:H    | 13       | 0.15          |
| (1,1378) | 1:341:A:VAL:HG23 | 1:345:A:GLN:H    | 13       | 0.15          |
| (1,872)  | 1:304:A:GLY:H    | 1:314:A:ILE:HB   | 15       | 0.15          |
| (1,734)  | 1:299:A:LYS:H    | 1:316:A:LEU:HD11 | 3        | 0.15          |
| (1,734)  | 1:299:A:LYS:H    | 1:316:A:LEU:HD12 | 3        | 0.15          |
| (1,734)  | 1:299:A:LYS:H    | 1:316:A:LEU:HD13 | 3        | 0.15          |
| (1,734)  | 1:299:A:LYS:H    | 1:316:A:LEU:HD21 | 3        | 0.15          |
| (1,734)  | 1:299:A:LYS:H    | 1:316:A:LEU:HD22 | 3        | 0.15          |
| (1,734)  | 1:299:A:LYS:H    | 1:316:A:LEU:HD23 | 3        | 0.15          |
| (1,437)  | 1:282:A:VAL:HG11 | 1:379:A:MET:HA   | 1        | 0.15          |
| (1,437)  | 1:282:A:VAL:HG12 | 1:379:A:MET:HA   | 1        | 0.15          |
| (1,437)  | 1:282:A:VAL:HG13 | 1:379:A:MET:HA   | 1        | 0.15          |
| (1,437)  | 1:282:A:VAL:HG21 | 1:379:A:MET:HA   | 1        | 0.15          |
| (1,437)  | 1:282:A:VAL:HG22 | 1:379:A:MET:HA   | 1        | 0.15          |
| (1,437)  | 1:282:A:VAL:HG23 | 1:379:A:MET:HA   | 1        | 0.15          |
| (4,51)   | 1:383:A:LYS:H    | 1:380:A:PRO:O    | 5        | 0.14          |
| (4,51)   | 1:383:A:LYS:H    | 1:380:A:PRO:O    | 10       | 0.14          |
| (4,14)   | 1:350:A:SER:N    | 1:290:A:THR:O    | 11       | 0.14          |
| (4,13)   | 1:348:A:GLY:O    | 1:292:A:VAL:N    | 7        | 0.14          |
| (4,13)   | 1:348:A:GLY:O    | 1:292:A:VAL:N    | 10       | 0.14          |
| (4,13)   | 1:348:A:GLY:O    | 1:292:A:VAL:N    | 12       | 0.14          |
| (4,12)   | 1:299:A:LYS:O    | 1:317:A:ILE:N    | 5        | 0.14          |
| (4,12)   | 1:299:A:LYS:O    | 1:317:A:ILE:N    | 11       | 0.14          |
| (4,10)   | 1:316:A:LEU:O    | 1:325:A:GLN:N    | 4        | 0.14          |
| (4,6)    | 1:366:A:MET:O    | 1:324:A:ARG:N    | 14       | 0.14          |
| (4,5)    | 1:366:A:MET:N    | 1:324:A:ARG:O    | 14       | 0.14          |
| (4,4)    | 1:364:A:GLN:O    | 1:326:A:TRP:N    | 15       | 0.14          |
| (2,1)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 9        | 0.14          |
| (2,1)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 14       | 0.14          |
| (1,3471) | 1:492:A:ILE:HG21 | 1:493:A:LYS:HG2  | 11       | 0.14          |
| (1,3471) | 1:492:A:ILE:HG21 | 1:493:A:LYS:HG3  | 11       | 0.14          |
| (1,3471) | 1:492:A:ILE:HG22 | 1:493:A:LYS:HG2  | 11       | 0.14          |
| (1,3471) | 1:492:A:ILE:HG22 | 1:493:A:LYS:HG3  | 11       | 0.14          |
| (1,3471) | 1:492:A:ILE:HG23 | 1:493:A:LYS:HG2  | 11       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3471) | 1:492:A:ILE:HG23 | 1:493:A:LYS:HG3  | 11       | 0.14          |
| (1,3467) | 1:492:A:ILE:HD11 | 1:493:A:LYS:H    | 9        | 0.14          |
| (1,3467) | 1:492:A:ILE:HD12 | 1:493:A:LYS:H    | 9        | 0.14          |
| (1,3467) | 1:492:A:ILE:HD13 | 1:493:A:LYS:H    | 9        | 0.14          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG11 | 6        | 0.14          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG12 | 6        | 0.14          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG13 | 6        | 0.14          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG21 | 6        | 0.14          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG22 | 6        | 0.14          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG23 | 6        | 0.14          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG11 | 11       | 0.14          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG12 | 11       | 0.14          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG13 | 11       | 0.14          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG21 | 11       | 0.14          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG22 | 11       | 0.14          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG23 | 11       | 0.14          |
| (1,2798) | 1:451:A:GLU:H    | 1:461:A:VAL:HG11 | 11       | 0.14          |
| (1,2798) | 1:451:A:GLU:H    | 1:461:A:VAL:HG12 | 11       | 0.14          |
| (1,2798) | 1:451:A:GLU:H    | 1:461:A:VAL:HG13 | 11       | 0.14          |
| (1,2798) | 1:451:A:GLU:H    | 1:461:A:VAL:HG21 | 11       | 0.14          |
| (1,2798) | 1:451:A:GLU:H    | 1:461:A:VAL:HG22 | 11       | 0.14          |
| (1,2798) | 1:451:A:GLU:H    | 1:461:A:VAL:HG23 | 11       | 0.14          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD11 | 15       | 0.14          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD12 | 15       | 0.14          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD13 | 15       | 0.14          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD21 | 15       | 0.14          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD22 | 15       | 0.14          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD23 | 15       | 0.14          |
| (1,1997) | 1:410:A:LEU:HD11 | 1:478:A:TRP:HE1  | 1        | 0.14          |
| (1,1997) | 1:410:A:LEU:HD12 | 1:478:A:TRP:HE1  | 1        | 0.14          |
| (1,1997) | 1:410:A:LEU:HD13 | 1:478:A:TRP:HE1  | 1        | 0.14          |
| (1,1997) | 1:410:A:LEU:HD21 | 1:478:A:TRP:HE1  | 1        | 0.14          |
| (1,1997) | 1:410:A:LEU:HD22 | 1:478:A:TRP:HE1  | 1        | 0.14          |
| (1,1997) | 1:410:A:LEU:HD23 | 1:478:A:TRP:HE1  | 1        | 0.14          |
| (1,1474) | 1:357:A:THR:HA   | 1:357:A:THR:HG21 | 2        | 0.14          |
| (1,1474) | 1:357:A:THR:HA   | 1:357:A:THR:HG22 | 2        | 0.14          |
| (1,1474) | 1:357:A:THR:HA   | 1:357:A:THR:HG23 | 2        | 0.14          |
| (1,1474) | 1:357:A:THR:HA   | 1:357:A:THR:HG21 | 10       | 0.14          |
| (1,1474) | 1:357:A:THR:HA   | 1:357:A:THR:HG22 | 10       | 0.14          |
| (1,1474) | 1:357:A:THR:HA   | 1:357:A:THR:HG23 | 10       | 0.14          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD11 | 9        | 0.14          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD12 | 9        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD13 | 9        | 0.14          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD21 | 9        | 0.14          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD22 | 9        | 0.14          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD23 | 9        | 0.14          |
| (1,1094) | 1:323:A:HIS:HD2  | 1:324:A:ARG:H    | 14       | 0.14          |
| (1,872)  | 1:304:A:GLY:H    | 1:314:A:ILE:HB   | 2        | 0.14          |
| (1,872)  | 1:304:A:GLY:H    | 1:314:A:ILE:HB   | 4        | 0.14          |
| (1,872)  | 1:304:A:GLY:H    | 1:314:A:ILE:HB   | 8        | 0.14          |
| (1,419)  | 1:282:A:VAL:HG11 | 1:283:A:ASP:HA   | 2        | 0.14          |
| (1,419)  | 1:282:A:VAL:HG12 | 1:283:A:ASP:HA   | 2        | 0.14          |
| (1,419)  | 1:282:A:VAL:HG13 | 1:283:A:ASP:HA   | 2        | 0.14          |
| (1,15)   | 1:253:A:HIS:HA   | 1:253:A:HIS:HD2  | 4        | 0.14          |
| (1,4)    | 1:252:A:GLU:HA   | 1:252:A:GLU:HG2  | 8        | 0.14          |
| (1,4)    | 1:252:A:GLU:HA   | 1:252:A:GLU:HG3  | 8        | 0.14          |
| (4,51)   | 1:383:A:LYS:H    | 1:380:A:PRO:O    | 12       | 0.13          |
| (4,21)   | 1:471:A:ILE:N    | 1:463:A:TYR:O    | 8        | 0.13          |
| (4,13)   | 1:348:A:GLY:O    | 1:292:A:VAL:N    | 1        | 0.13          |
| (4,10)   | 1:316:A:LEU:O    | 1:325:A:GLN:N    | 3        | 0.13          |
| (4,7)    | 1:314:A:ILE:N    | 1:327:A:TYR:O    | 13       | 0.13          |
| (4,6)    | 1:366:A:MET:O    | 1:324:A:ARG:N    | 7        | 0.13          |
| (4,5)    | 1:366:A:MET:N    | 1:324:A:ARG:O    | 4        | 0.13          |
| (4,5)    | 1:366:A:MET:N    | 1:324:A:ARG:O    | 8        | 0.13          |
| (4,5)    | 1:366:A:MET:N    | 1:324:A:ARG:O    | 12       | 0.13          |
| (4,5)    | 1:366:A:MET:N    | 1:324:A:ARG:O    | 13       | 0.13          |
| (4,4)    | 1:364:A:GLN:O    | 1:326:A:TRP:N    | 9        | 0.13          |
| (2,1)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 8        | 0.13          |
| (2,1)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 15       | 0.13          |
| (1,3333) | 1:478:A:TRP:HD1  | 1:485:A:LEU:HG   | 5        | 0.13          |
| (1,2666) | 1:440:A:VAL:HG11 | 1:442:A:LYS:H    | 3        | 0.13          |
| (1,2666) | 1:440:A:VAL:HG12 | 1:442:A:LYS:H    | 3        | 0.13          |
| (1,2666) | 1:440:A:VAL:HG13 | 1:442:A:LYS:H    | 3        | 0.13          |
| (1,2666) | 1:440:A:VAL:HG21 | 1:442:A:LYS:H    | 3        | 0.13          |
| (1,2666) | 1:440:A:VAL:HG22 | 1:442:A:LYS:H    | 3        | 0.13          |
| (1,2666) | 1:440:A:VAL:HG23 | 1:442:A:LYS:H    | 3        | 0.13          |
| (1,2446) | 1:426:A:THR:HA   | 1:474:A:PRO:HG3  | 1        | 0.13          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD11 | 15       | 0.13          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD12 | 15       | 0.13          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD13 | 15       | 0.13          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD21 | 15       | 0.13          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD22 | 15       | 0.13          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD23 | 15       | 0.13          |
| (1,1771) | 1:389:A:LYS:HA   | 1:389:A:LYS:HD2  | 1        | 0.13          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1771) | 1:389:A:LYS:HA  | 1:389:A:LYS:HD3  | 1        | 0.13          |
| (1,1474) | 1:357:A:THR:HA  | 1:357:A:THR:HG21 | 14       | 0.13          |
| (1,1474) | 1:357:A:THR:HA  | 1:357:A:THR:HG22 | 14       | 0.13          |
| (1,1474) | 1:357:A:THR:HA  | 1:357:A:THR:HG23 | 14       | 0.13          |
| (1,1172) | 1:327:A:TYR:H   | 1:330:A:LEU:HD11 | 5        | 0.13          |
| (1,1172) | 1:327:A:TYR:H   | 1:330:A:LEU:HD12 | 5        | 0.13          |
| (1,1172) | 1:327:A:TYR:H   | 1:330:A:LEU:HD13 | 5        | 0.13          |
| (1,1172) | 1:327:A:TYR:H   | 1:330:A:LEU:HD21 | 5        | 0.13          |
| (1,1172) | 1:327:A:TYR:H   | 1:330:A:LEU:HD22 | 5        | 0.13          |
| (1,1172) | 1:327:A:TYR:H   | 1:330:A:LEU:HD23 | 5        | 0.13          |
| (1,872)  | 1:304:A:GLY:H   | 1:314:A:ILE:HB   | 10       | 0.13          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD11 | 11       | 0.13          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD12 | 11       | 0.13          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD13 | 11       | 0.13          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD21 | 11       | 0.13          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD22 | 11       | 0.13          |
| (1,735)  | 1:299:A:LYS:HB2 | 1:316:A:LEU:HD23 | 11       | 0.13          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD11 | 11       | 0.13          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD12 | 11       | 0.13          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD13 | 11       | 0.13          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD21 | 11       | 0.13          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD22 | 11       | 0.13          |
| (1,735)  | 1:299:A:LYS:HB3 | 1:316:A:LEU:HD23 | 11       | 0.13          |
| (1,379)  | 1:278:A:MET:H   | 1:278:A:MET:HE1  | 2        | 0.13          |
| (1,379)  | 1:278:A:MET:H   | 1:278:A:MET:HE2  | 2        | 0.13          |
| (1,379)  | 1:278:A:MET:H   | 1:278:A:MET:HE3  | 2        | 0.13          |
| (1,378)  | 1:277:A:GLY:H   | 1:278:A:MET:H    | 12       | 0.13          |
| (1,137)  | 1:257:A:TRP:HZ2 | 1:292:A:VAL:HG11 | 2        | 0.13          |
| (1,137)  | 1:257:A:TRP:HZ2 | 1:292:A:VAL:HG12 | 2        | 0.13          |
| (1,137)  | 1:257:A:TRP:HZ2 | 1:292:A:VAL:HG13 | 2        | 0.13          |
| (1,137)  | 1:257:A:TRP:HZ2 | 1:292:A:VAL:HG21 | 2        | 0.13          |
| (1,137)  | 1:257:A:TRP:HZ2 | 1:292:A:VAL:HG22 | 2        | 0.13          |
| (1,137)  | 1:257:A:TRP:HZ2 | 1:292:A:VAL:HG23 | 2        | 0.13          |
| (4,51)   | 1:383:A:LYS:H   | 1:380:A:PRO:O    | 6        | 0.12          |
| (4,51)   | 1:383:A:LYS:H   | 1:380:A:PRO:O    | 15       | 0.12          |
| (4,22)   | 1:461:A:VAL:N   | 1:473:A:LEU:O    | 2        | 0.12          |
| (4,22)   | 1:461:A:VAL:N   | 1:473:A:LEU:O    | 4        | 0.12          |
| (4,22)   | 1:461:A:VAL:N   | 1:473:A:LEU:O    | 5        | 0.12          |
| (4,16)   | 1:453:A:MET:N   | 1:460:A:TRP:O    | 2        | 0.12          |
| (4,15)   | 1:383:A:LYS:N   | 1:380:A:PRO:O    | 4        | 0.12          |
| (4,15)   | 1:383:A:LYS:N   | 1:380:A:PRO:O    | 9        | 0.12          |
| (4,13)   | 1:348:A:GLY:O   | 1:292:A:VAL:N    | 3        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (4,10)   | 1:316:A:LEU:O    | 1:325:A:GLN:N    | 10       | 0.12          |
| (2,1)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 7        | 0.12          |
| (1,3333) | 1:478:A:TRP:HD1  | 1:485:A:LEU:HG   | 12       | 0.12          |
| (1,3333) | 1:478:A:TRP:HD1  | 1:485:A:LEU:HG   | 15       | 0.12          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD11 | 3        | 0.12          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD12 | 3        | 0.12          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD13 | 3        | 0.12          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD21 | 3        | 0.12          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD22 | 3        | 0.12          |
| (1,3283) | 1:477:A:THR:H    | 1:485:A:LEU:HD23 | 3        | 0.12          |
| (1,3159) | 1:470:A:ARG:H    | 1:470:A:ARG:HD2  | 3        | 0.12          |
| (1,3159) | 1:470:A:ARG:H    | 1:470:A:ARG:HD3  | 3        | 0.12          |
| (1,3159) | 1:470:A:ARG:H    | 1:470:A:ARG:HD2  | 12       | 0.12          |
| (1,3159) | 1:470:A:ARG:H    | 1:470:A:ARG:HD3  | 12       | 0.12          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG11 | 4        | 0.12          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG12 | 4        | 0.12          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG13 | 4        | 0.12          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG21 | 4        | 0.12          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG22 | 4        | 0.12          |
| (1,2988) | 1:459:A:VAL:H    | 1:475:A:VAL:HG23 | 4        | 0.12          |
| (1,2817) | 1:452:A:VAL:H    | 1:461:A:VAL:HG11 | 1        | 0.12          |
| (1,2817) | 1:452:A:VAL:H    | 1:461:A:VAL:HG12 | 1        | 0.12          |
| (1,2817) | 1:452:A:VAL:H    | 1:461:A:VAL:HG13 | 1        | 0.12          |
| (1,2817) | 1:452:A:VAL:H    | 1:461:A:VAL:HG21 | 1        | 0.12          |
| (1,2817) | 1:452:A:VAL:H    | 1:461:A:VAL:HG22 | 1        | 0.12          |
| (1,2817) | 1:452:A:VAL:H    | 1:461:A:VAL:HG23 | 1        | 0.12          |
| (1,1984) | 1:410:A:LEU:HD11 | 1:411:A:TYR:H    | 12       | 0.12          |
| (1,1984) | 1:410:A:LEU:HD12 | 1:411:A:TYR:H    | 12       | 0.12          |
| (1,1984) | 1:410:A:LEU:HD13 | 1:411:A:TYR:H    | 12       | 0.12          |
| (1,1984) | 1:410:A:LEU:HD21 | 1:411:A:TYR:H    | 12       | 0.12          |
| (1,1984) | 1:410:A:LEU:HD22 | 1:411:A:TYR:H    | 12       | 0.12          |
| (1,1984) | 1:410:A:LEU:HD23 | 1:411:A:TYR:H    | 12       | 0.12          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD11 | 4        | 0.12          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD12 | 4        | 0.12          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD13 | 4        | 0.12          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD21 | 4        | 0.12          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD22 | 4        | 0.12          |
| (1,1172) | 1:327:A:TYR:H    | 1:330:A:LEU:HD23 | 4        | 0.12          |
| (1,1046) | 1:318:A:GLU:HA   | 1:320:A:ASP:H    | 9        | 0.12          |
| (1,911)  | 1:310:A:GLY:H    | 1:311:A:GLY:H    | 7        | 0.12          |
| (1,872)  | 1:304:A:GLY:H    | 1:314:A:ILE:HB   | 7        | 0.12          |
| (4,51)   | 1:383:A:LYS:H    | 1:380:A:PRO:O    | 3        | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (4,51)   | 1:383:A:LYS:H   | 1:380:A:PRO:O    | 4        | 0.11          |
| (4,22)   | 1:461:A:VAL:N   | 1:473:A:LEU:O    | 13       | 0.11          |
| (4,21)   | 1:471:A:ILE:N   | 1:463:A:TYR:O    | 1        | 0.11          |
| (4,13)   | 1:348:A:GLY:O   | 1:292:A:VAL:N    | 11       | 0.11          |
| (4,13)   | 1:348:A:GLY:O   | 1:292:A:VAL:N    | 14       | 0.11          |
| (4,13)   | 1:348:A:GLY:O   | 1:292:A:VAL:N    | 15       | 0.11          |
| (4,12)   | 1:299:A:LYS:O   | 1:317:A:ILE:N    | 3        | 0.11          |
| (4,12)   | 1:299:A:LYS:O   | 1:317:A:ILE:N    | 12       | 0.11          |
| (4,10)   | 1:316:A:LEU:O   | 1:325:A:GLN:N    | 13       | 0.11          |
| (4,5)    | 1:366:A:MET:N   | 1:324:A:ARG:O    | 10       | 0.11          |
| (4,5)    | 1:366:A:MET:N   | 1:324:A:ARG:O    | 15       | 0.11          |
| (2,6)    | 1:362:A:HIS:ND1 | 2:501:A:ZN:ZN    | 1        | 0.11          |
| (2,6)    | 1:362:A:HIS:ND1 | 2:501:A:ZN:ZN    | 2        | 0.11          |
| (2,6)    | 1:362:A:HIS:ND1 | 2:501:A:ZN:ZN    | 4        | 0.11          |
| (2,6)    | 1:362:A:HIS:ND1 | 2:501:A:ZN:ZN    | 8        | 0.11          |
| (2,6)    | 1:362:A:HIS:ND1 | 2:501:A:ZN:ZN    | 9        | 0.11          |
| (2,6)    | 1:362:A:HIS:ND1 | 2:501:A:ZN:ZN    | 12       | 0.11          |
| (2,6)    | 1:362:A:HIS:ND1 | 2:501:A:ZN:ZN    | 14       | 0.11          |
| (2,1)    | 1:279:A:HIS:NE2 | 2:501:A:ZN:ZN    | 5        | 0.11          |
| (2,1)    | 1:279:A:HIS:NE2 | 2:501:A:ZN:ZN    | 10       | 0.11          |
| (1,3450) | 1:491:A:THR:H   | 1:492:A:ILE:HG12 | 13       | 0.11          |
| (1,3450) | 1:491:A:THR:H   | 1:492:A:ILE:HG13 | 13       | 0.11          |
| (1,3333) | 1:478:A:TRP:HD1 | 1:485:A:LEU:HG   | 2        | 0.11          |
| (1,3333) | 1:478:A:TRP:HD1 | 1:485:A:LEU:HG   | 9        | 0.11          |
| (1,3268) | 1:476:A:ARG:H   | 1:489:A:TRP:HE1  | 10       | 0.11          |
| (1,2988) | 1:459:A:VAL:H   | 1:475:A:VAL:HG11 | 12       | 0.11          |
| (1,2988) | 1:459:A:VAL:H   | 1:475:A:VAL:HG12 | 12       | 0.11          |
| (1,2988) | 1:459:A:VAL:H   | 1:475:A:VAL:HG13 | 12       | 0.11          |
| (1,2988) | 1:459:A:VAL:H   | 1:475:A:VAL:HG21 | 12       | 0.11          |
| (1,2988) | 1:459:A:VAL:H   | 1:475:A:VAL:HG22 | 12       | 0.11          |
| (1,2988) | 1:459:A:VAL:H   | 1:475:A:VAL:HG23 | 12       | 0.11          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG11 | 3        | 0.11          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG12 | 3        | 0.11          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG13 | 3        | 0.11          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG21 | 3        | 0.11          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG22 | 3        | 0.11          |
| (1,2799) | 1:451:A:GLU:HA  | 1:461:A:VAL:HG23 | 3        | 0.11          |
| (1,2697) | 1:444:A:GLY:H   | 1:445:A:GLN:HA   | 5        | 0.11          |
| (1,2487) | 1:427:A:ARG:HE  | 1:460:A:TRP:HZ3  | 13       | 0.11          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD11 | 12       | 0.11          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD12 | 12       | 0.11          |
| (1,2352) | 1:424:A:ILE:H   | 1:441:A:LEU:HD13 | 12       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD21 | 12       | 0.11          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD22 | 12       | 0.11          |
| (1,2352) | 1:424:A:ILE:H    | 1:441:A:LEU:HD23 | 12       | 0.11          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD11 | 4        | 0.11          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD12 | 4        | 0.11          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD13 | 4        | 0.11          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD21 | 4        | 0.11          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD22 | 4        | 0.11          |
| (1,2247) | 1:420:A:PRO:HB2  | 1:441:A:LEU:HD23 | 4        | 0.11          |
| (1,1940) | 1:407:A:TYR:HB3  | 1:409:A:THR:H    | 15       | 0.11          |
| (1,1865) | 1:404:A:THR:HA   | 1:409:A:THR:H    | 15       | 0.11          |
| (1,1780) | 1:397:A:THR:HA   | 1:397:A:THR:HG21 | 2        | 0.11          |
| (1,1780) | 1:397:A:THR:HA   | 1:397:A:THR:HG22 | 2        | 0.11          |
| (1,1780) | 1:397:A:THR:HA   | 1:397:A:THR:HG23 | 2        | 0.11          |
| (1,1780) | 1:397:A:THR:HA   | 1:397:A:THR:HG21 | 5        | 0.11          |
| (1,1780) | 1:397:A:THR:HA   | 1:397:A:THR:HG22 | 5        | 0.11          |
| (1,1780) | 1:397:A:THR:HA   | 1:397:A:THR:HG23 | 5        | 0.11          |
| (1,1780) | 1:397:A:THR:HA   | 1:397:A:THR:HG21 | 12       | 0.11          |
| (1,1780) | 1:397:A:THR:HA   | 1:397:A:THR:HG22 | 12       | 0.11          |
| (1,1780) | 1:397:A:THR:HA   | 1:397:A:THR:HG23 | 12       | 0.11          |
| (1,1210) | 1:330:A:LEU:H    | 1:332:A:LYS:H    | 2        | 0.11          |
| (1,1209) | 1:330:A:LEU:HD11 | 1:331:A:SER:H    | 14       | 0.11          |
| (1,1209) | 1:330:A:LEU:HD12 | 1:331:A:SER:H    | 14       | 0.11          |
| (1,1209) | 1:330:A:LEU:HD13 | 1:331:A:SER:H    | 14       | 0.11          |
| (1,1209) | 1:330:A:LEU:HD21 | 1:331:A:SER:H    | 14       | 0.11          |
| (1,1209) | 1:330:A:LEU:HD22 | 1:331:A:SER:H    | 14       | 0.11          |
| (1,1209) | 1:330:A:LEU:HD23 | 1:331:A:SER:H    | 14       | 0.11          |
| (1,1046) | 1:318:A:GLU:HA   | 1:320:A:ASP:H    | 10       | 0.11          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD11 | 12       | 0.11          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD12 | 12       | 0.11          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD13 | 12       | 0.11          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD21 | 12       | 0.11          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD22 | 12       | 0.11          |
| (1,735)  | 1:299:A:LYS:HB2  | 1:316:A:LEU:HD23 | 12       | 0.11          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD11 | 12       | 0.11          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD12 | 12       | 0.11          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD13 | 12       | 0.11          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD21 | 12       | 0.11          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD22 | 12       | 0.11          |
| (1,735)  | 1:299:A:LYS:HB3  | 1:316:A:LEU:HD23 | 12       | 0.11          |
| (1,718)  | 1:298:A:GLY:H    | 1:342:A:LYS:HG2  | 4        | 0.11          |
| (1,718)  | 1:298:A:GLY:H    | 1:342:A:LYS:HG3  | 4        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,649)  | 1:295:A:ILE:HG21 | 1:297:A:SER:H    | 9        | 0.11          |
| (1,649)  | 1:295:A:ILE:HG22 | 1:297:A:SER:H    | 9        | 0.11          |
| (1,649)  | 1:295:A:ILE:HG23 | 1:297:A:SER:H    | 9        | 0.11          |
| (1,379)  | 1:278:A:MET:H    | 1:278:A:MET:HE1  | 5        | 0.11          |
| (1,379)  | 1:278:A:MET:H    | 1:278:A:MET:HE2  | 5        | 0.11          |
| (1,379)  | 1:278:A:MET:H    | 1:278:A:MET:HE3  | 5        | 0.11          |
| (4,51)   | 1:383:A:LYS:H    | 1:380:A:PRO:O    | 1        | 0.1           |
| (4,22)   | 1:461:A:VAL:N    | 1:473:A:LEU:O    | 6        | 0.1           |
| (4,21)   | 1:471:A:ILE:N    | 1:463:A:TYR:O    | 10       | 0.1           |
| (4,16)   | 1:453:A:MET:N    | 1:460:A:TRP:O    | 15       | 0.1           |
| (4,13)   | 1:348:A:GLY:O    | 1:292:A:VAL:N    | 2        | 0.1           |
| (4,13)   | 1:348:A:GLY:O    | 1:292:A:VAL:N    | 13       | 0.1           |
| (4,10)   | 1:316:A:LEU:O    | 1:325:A:GLN:N    | 5        | 0.1           |
| (4,10)   | 1:316:A:LEU:O    | 1:325:A:GLN:N    | 15       | 0.1           |
| (2,6)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 3        | 0.1           |
| (2,6)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 5        | 0.1           |
| (2,6)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 6        | 0.1           |
| (2,6)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 7        | 0.1           |
| (2,6)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 10       | 0.1           |
| (2,6)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 11       | 0.1           |
| (2,6)    | 1:362:A:HIS:ND1  | 2:501:A:ZN:ZN    | 15       | 0.1           |
| (2,4)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 3        | 0.1           |
| (2,4)    | 1:279:A:HIS:NE2  | 2:501:A:ZN:ZN    | 13       | 0.1           |
| (1,2678) | 1:441:A:LEU:HG   | 1:447:A:ILE:HG21 | 12       | 0.1           |
| (1,2678) | 1:441:A:LEU:HG   | 1:447:A:ILE:HG22 | 12       | 0.1           |
| (1,2678) | 1:441:A:LEU:HG   | 1:447:A:ILE:HG23 | 12       | 0.1           |
| (1,2446) | 1:426:A:THR:HA   | 1:474:A:PRO:HG3  | 6        | 0.1           |
| (1,1779) | 1:396:A:PRO:HA   | 1:397:A:THR:H    | 4        | 0.1           |
| (1,1747) | 1:384:A:SER:H    | 1:387:A:TYR:H    | 9        | 0.1           |
| (1,1269) | 1:332:A:LYS:HG2  | 1:349:A:TRP:H    | 5        | 0.1           |
| (1,1269) | 1:332:A:LYS:HG3  | 1:349:A:TRP:H    | 5        | 0.1           |
| (1,1088) | 1:322:A:VAL:HG11 | 1:368:A:ASN:HA   | 14       | 0.1           |
| (1,1088) | 1:322:A:VAL:HG12 | 1:368:A:ASN:HA   | 14       | 0.1           |
| (1,1088) | 1:322:A:VAL:HG13 | 1:368:A:ASN:HA   | 14       | 0.1           |
| (1,1088) | 1:322:A:VAL:HG21 | 1:368:A:ASN:HA   | 14       | 0.1           |
| (1,1088) | 1:322:A:VAL:HG22 | 1:368:A:ASN:HA   | 14       | 0.1           |
| (1,1088) | 1:322:A:VAL:HG23 | 1:368:A:ASN:HA   | 14       | 0.1           |
| (1,872)  | 1:304:A:GLY:H    | 1:314:A:ILE:HB   | 3        | 0.1           |

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

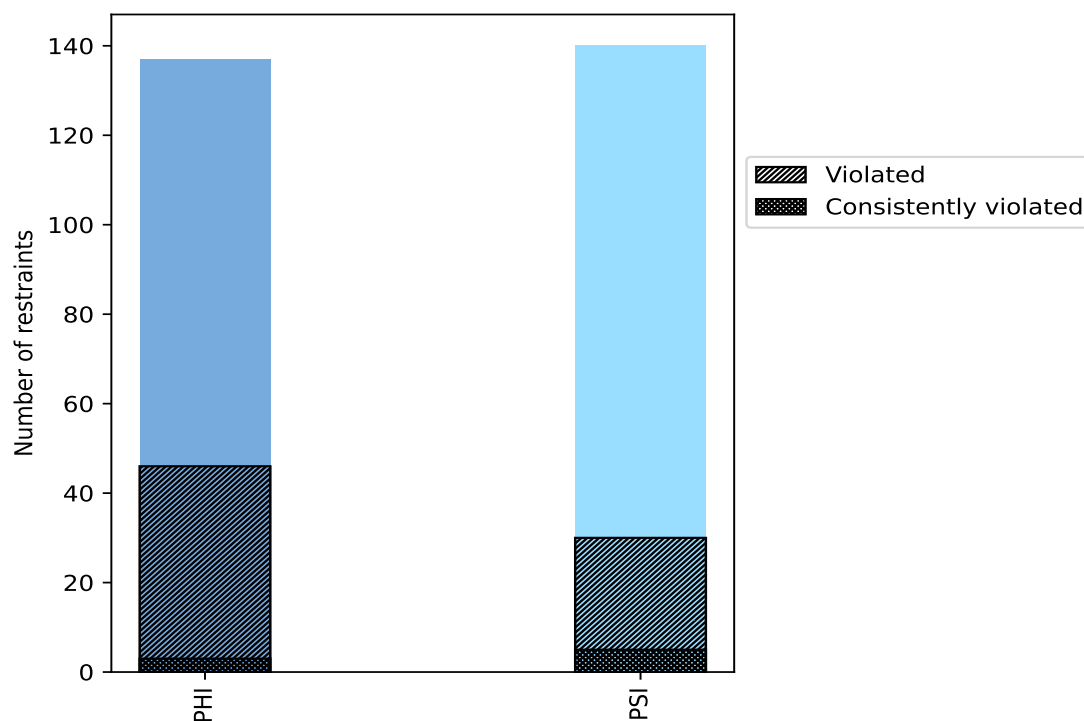
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 137   | 49.5           | 46                    | 33.6           | 16.6           | 3                                  | 2.2            | 1.1            |
| PSI        | 140   | 50.5           | 30                    | 21.4           | 10.8           | 5                                  | 3.6            | 1.8            |
| Total      | 277   | 100.0          | 76                    | 27.4           | 27.4           | 8                                  | 2.9            | 2.9            |

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

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



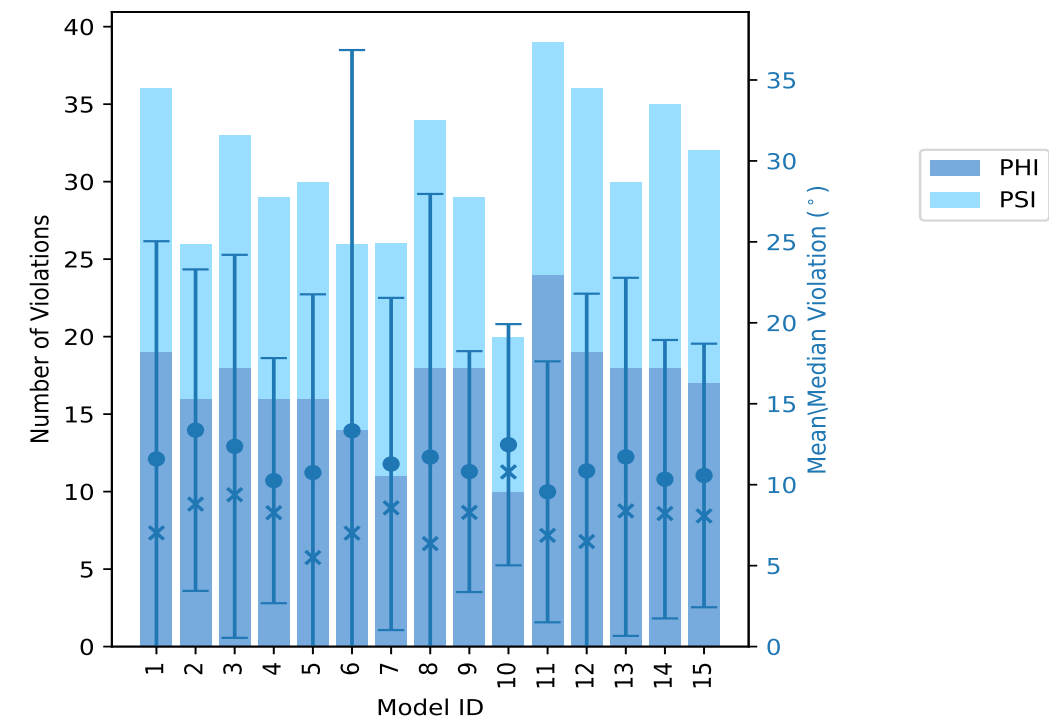
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 19                   | 17  | 36    | 11.59    | 73.38   | 13.45  | 7.02       |
| 2        | 16                   | 10  | 26    | 13.37    | 42.3    | 9.93   | 8.8        |
| 3        | 18                   | 15  | 33    | 12.37    | 57.72   | 11.83  | 9.38       |
| 4        | 16                   | 13  | 29    | 10.25    | 29.84   | 7.57   | 8.27       |
| 5        | 16                   | 14  | 30    | 10.75    | 43.81   | 11.01  | 5.5        |
| 6        | 14                   | 12  | 26    | 13.33    | 127.09  | 23.52  | 7.01       |
| 7        | 11                   | 15  | 26    | 11.28    | 50.36   | 10.26  | 8.57       |
| 8        | 18                   | 16  | 34    | 11.71    | 81.39   | 16.25  | 6.36       |
| 9        | 18                   | 11  | 29    | 10.81    | 29.06   | 7.44   | 8.29       |
| 10       | 10                   | 10  | 20    | 12.47    | 28.3    | 7.45   | 10.79      |
| 11       | 24                   | 15  | 39    | 9.56     | 29.49   | 8.06   | 6.87       |
| 12       | 19                   | 17  | 36    | 10.85    | 42.29   | 10.95  | 6.49       |
| 13       | 18                   | 12  | 30    | 11.72    | 48.46   | 11.06  | 8.38       |
| 14       | 18                   | 17  | 35    | 10.34    | 35.66   | 8.6    | 8.22       |
| 15       | 17                   | 15  | 32    | 10.57    | 31.5    | 8.14   | 8.07       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

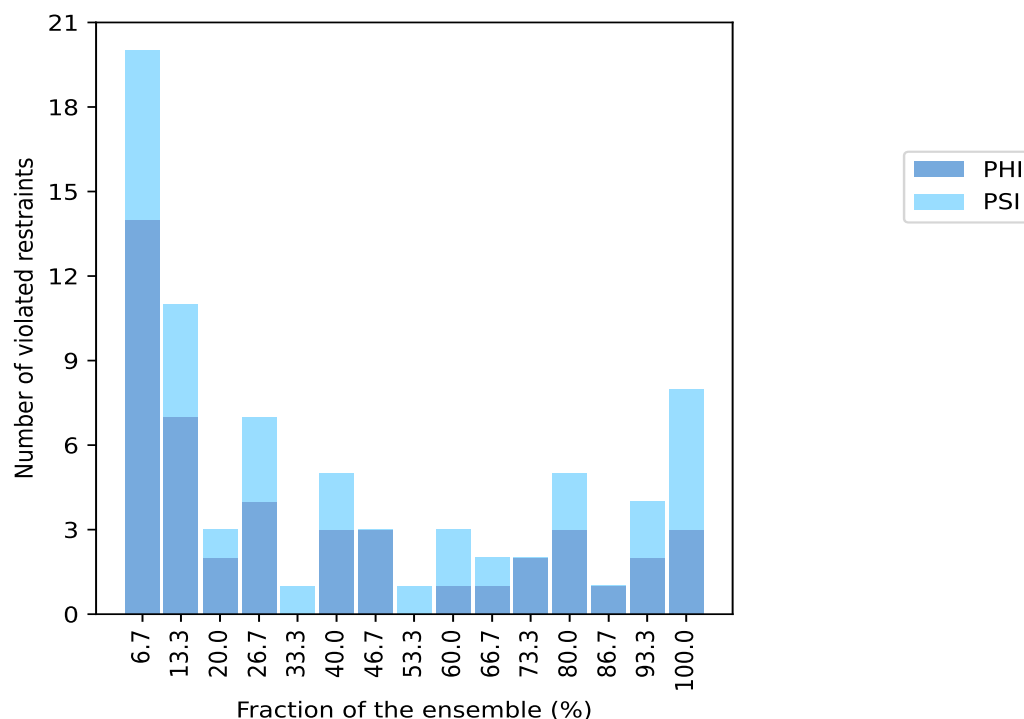
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |
| 14                            | 6   | 20    | 1                        | 6.7   |
| 7                             | 4   | 11    | 2                        | 13.3  |
| 2                             | 1   | 3     | 3                        | 20.0  |
| 4                             | 3   | 7     | 4                        | 26.7  |
| 0                             | 1   | 1     | 5                        | 33.3  |
| 3                             | 2   | 5     | 6                        | 40.0  |
| 3                             | 0   | 3     | 7                        | 46.7  |
| 0                             | 1   | 1     | 8                        | 53.3  |
| 1                             | 2   | 3     | 9                        | 60.0  |
| 1                             | 1   | 2     | 10                       | 66.7  |
| 2                             | 0   | 2     | 11                       | 73.3  |
| 3                             | 2   | 5     | 12                       | 80.0  |
| 1                             | 0   | 1     | 13                       | 86.7  |
| 2                             | 2   | 4     | 14                       | 93.3  |
| 3                             | 5   | 8     | 15                       | 100.0 |

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

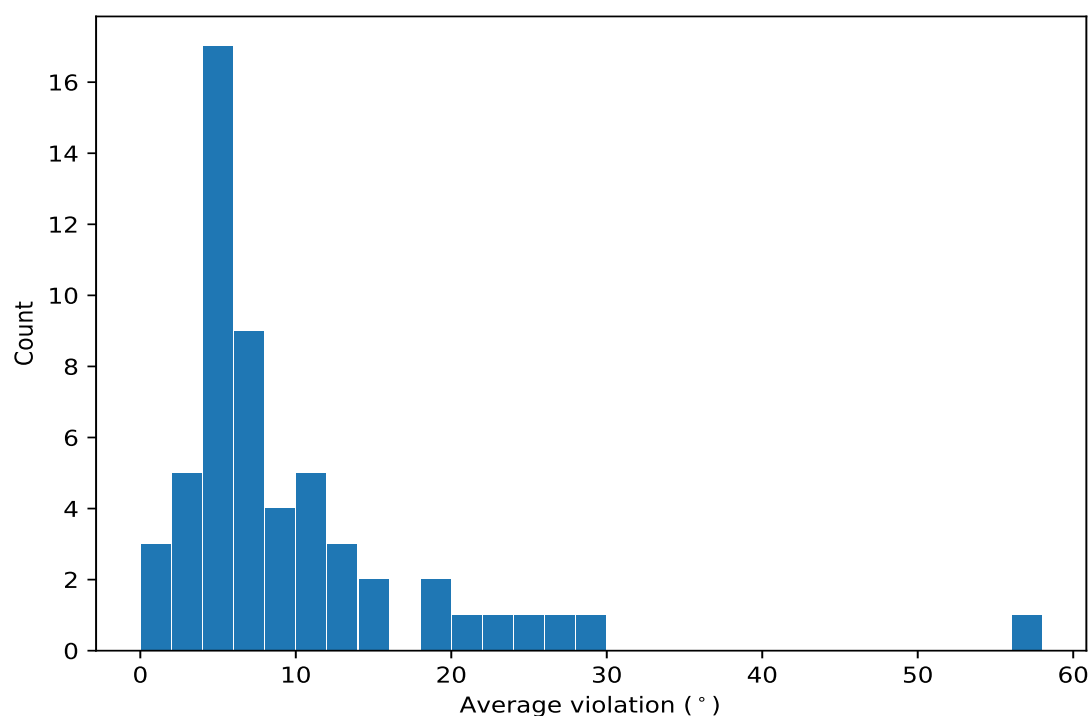
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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 |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 15                  | 21.88 | 6.5             | 20.03  |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 15                  | 18.25 | 7.06            | 18.64  |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 15                  | 15.57 | 6.64            | 16.6   |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 15                  | 13.27 | 3.76            | 12.7   |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 15                  | 10.0  | 4.53            | 9.6    |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 15                  | 8.71  | 1.76            | 8.27   |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 15                  | 5.56  | 2.59            | 6.67   |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 15                  | 5.14  | 2.48            | 4.12   |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 14                  | 14.79 | 5.83            | 15.96  |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 14                  | 13.69 | 5.81            | 12.91  |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 14                  | 5.24  | 2.97            | 4.36   |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 14                  | 4.13  | 1.93            | 3.52   |
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 13                  | 26.65 | 15.1            | 27.37  |
| (1,127) | 1:370:A:PHE:C | 1:371:A:SER:N  | 1:371:A:SER:CA | 1:371:A:SER:C | 12                  | 28.2  | 10.13           | 29.26  |
| (1,262) | 1:481:A:SER:C | 1:482:A:THR:N  | 1:482:A:THR:CA | 1:482:A:THR:C | 12                  | 13.35 | 6.59            | 10.92  |
| (1,202) | 1:439:A:GLY:N | 1:439:A:GLY:CA | 1:439:A:GLY:C  | 1:440:A:VAL:N | 12                  | 8.74  | 7.35            | 7.52   |
| (1,254) | 1:477:A:THR:C | 1:478:A:TRP:N  | 1:478:A:TRP:CA | 1:478:A:TRP:C | 12                  | 7.26  | 2.77            | 7.07   |
| (1,273) | 1:490:A:GLY:N | 1:490:A:GLY:CA | 1:490:A:GLY:C  | 1:491:A:THR:N | 12                  | 5.69  | 2.83            | 5.24   |
| (1,111) | 1:352:A:SER:C | 1:353:A:THR:N  | 1:353:A:THR:CA | 1:353:A:THR:C | 11                  | 19.43 | 15.24           | 16.05  |
| (1,33)  | 1:295:A:ILE:C | 1:296:A:SER:N  | 1:296:A:SER:CA | 1:296:A:SER:C | 11                  | 6.87  | 3.69            | 6.18   |
| (1,176) | 1:416:A:ALA:C | 1:417:A:SER:N  | 1:417:A:SER:CA | 1:417:A:SER:C | 10                  | 10.51 | 5.06            | 10.28  |

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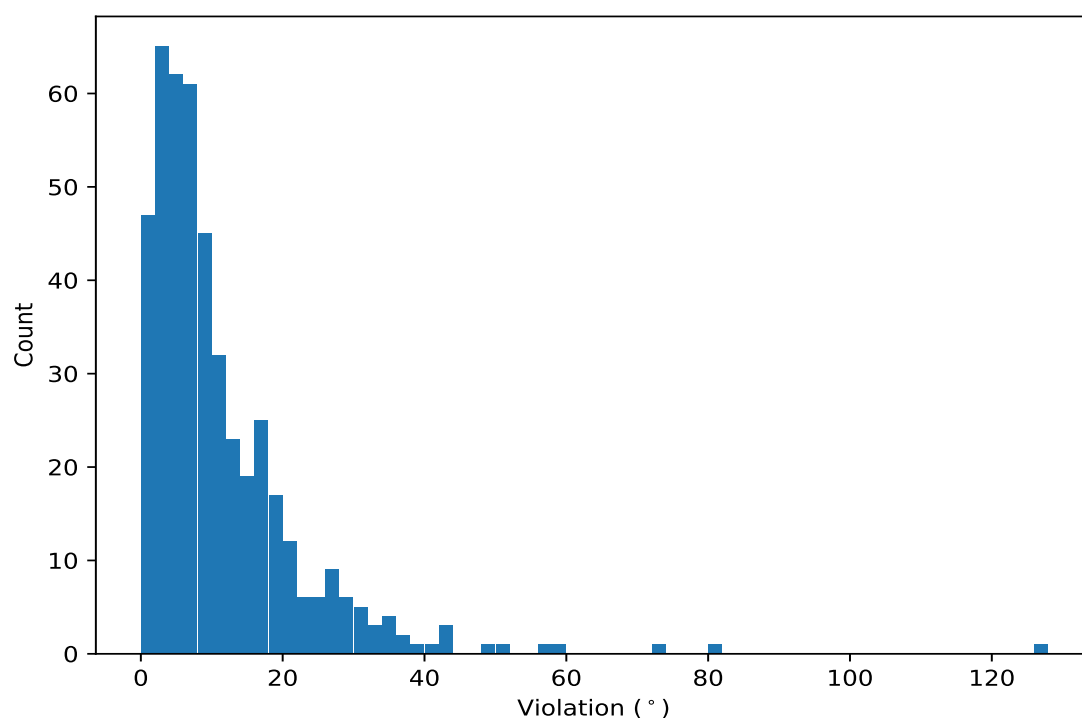
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,198) | 1:433:A:ARG:N | 1:433:A:ARG:CA | 1:433:A:ARG:C  | 1:434:A:SER:N | 10                  | 5.83  | 2.99            | 5.18   |
| (1,11)  | 1:277:A:GLY:C | 1:278:A:MET:N  | 1:278:A:MET:CA | 1:278:A:MET:C | 9                   | 10.59 | 6.11            | 8.22   |
| (1,155) | 1:402:A:TRP:N | 1:402:A:TRP:CA | 1:402:A:TRP:C  | 1:403:A:LYS:N | 9                   | 8.36  | 3.72            | 8.39   |
| (1,18)  | 1:281:A:GLY:N | 1:281:A:GLY:CA | 1:281:A:GLY:C  | 1:282:A:VAL:N | 9                   | 6.11  | 2.1             | 6.75   |
| (1,62)  | 1:321:A:GLY:N | 1:321:A:GLY:CA | 1:321:A:GLY:C  | 1:322:A:VAL:N | 8                   | 7.71  | 5.37            | 6.26   |
| (1,115) | 1:360:A:HIS:C | 1:361:A:LEU:N  | 1:361:A:LEU:CA | 1:361:A:LEU:C | 7                   | 24.98 | 6.53            | 26.92  |
| (1,15)  | 1:279:A:HIS:C | 1:280:A:TYR:N  | 1:280:A:TYR:CA | 1:280:A:TYR:C | 7                   | 7.28  | 3.03            | 6.52   |
| (1,247) | 1:472:A:TYR:C | 1:473:A:LEU:N  | 1:473:A:LEU:CA | 1:473:A:LEU:C | 7                   | 1.91  | 0.51            | 1.97   |
| (1,112) | 1:353:A:THR:N | 1:353:A:THR:CA | 1:353:A:THR:C  | 1:354:A:GLY:N | 6                   | 57.48 | 37.39           | 54.94  |
| (1,37)  | 1:298:A:GLY:C | 1:299:A:LYS:N  | 1:299:A:LYS:CA | 1:299:A:LYS:C | 6                   | 8.98  | 5.09            | 10.16  |
| (1,77)  | 1:332:A:LYS:C | 1:333:A:TYR:N  | 1:333:A:TYR:CA | 1:333:A:TYR:C | 6                   | 7.91  | 4.8             | 7.18   |
| (1,263) | 1:482:A:THR:N | 1:482:A:THR:CA | 1:482:A:THR:C  | 1:483:A:ASN:N | 6                   | 6.1   | 4.32            | 5.96   |
| (1,17)  | 1:280:A:TYR:C | 1:281:A:GLY:N  | 1:281:A:GLY:CA | 1:281:A:GLY:C | 6                   | 4.69  | 3.55            | 3.86   |
| (1,196) | 1:432:A:PHE:N | 1:432:A:PHE:CA | 1:432:A:PHE:C  | 1:433:A:ARG:N | 5                   | 3.52  | 1.52            | 2.99   |
| (1,113) | 1:356:A:SER:C | 1:357:A:THR:N  | 1:357:A:THR:CA | 1:357:A:THR:C | 4                   | 23.04 | 14.6            | 24.6   |
| (1,59)  | 1:319:A:ASN:C | 1:320:A:ASP:N  | 1:320:A:ASP:CA | 1:320:A:ASP:C | 4                   | 10.72 | 7.5             | 10.66  |
| (1,2)   | 1:259:A:ASN:N | 1:259:A:ASN:CA | 1:259:A:ASN:C  | 1:260:A:ASN:N | 4                   | 10.64 | 14.47           | 2.62   |
| (1,135) | 1:376:A:GLN:C | 1:377:A:ASP:N  | 1:377:A:ASP:CA | 1:377:A:ASP:C | 4                   | 4.84  | 2.07            | 4.46   |
| (1,154) | 1:401:A:GLY:C | 1:402:A:TRP:N  | 1:402:A:TRP:CA | 1:402:A:TRP:C | 4                   | 4.82  | 2.01            | 5.66   |
| (1,277) | 1:492:A:ILE:N | 1:492:A:ILE:CA | 1:492:A:ILE:C  | 1:493:A:LYS:N | 4                   | 4.81  | 4.94            | 2.46   |
| (1,151) | 1:386:A:GLY:N | 1:386:A:GLY:CA | 1:386:A:GLY:C  | 1:387:A:TYR:N | 4                   | 4.68  | 1.53            | 5.55   |
| (1,12)  | 1:278:A:MET:N | 1:278:A:MET:CA | 1:278:A:MET:C  | 1:279:A:HIS:N | 3                   | 4.71  | 4.53            | 1.55   |
| (1,21)  | 1:282:A:VAL:C | 1:283:A:ASP:N  | 1:283:A:ASP:CA | 1:283:A:ASP:C | 3                   | 3.92  | 1.47            | 3.17   |
| (1,187) | 1:423:A:ASP:C | 1:424:A:ILE:N  | 1:424:A:ILE:CA | 1:424:A:ILE:C | 3                   | 3.53  | 1.63            | 4.63   |
| (1,64)  | 1:324:A:ARG:N | 1:324:A:ARG:CA | 1:324:A:ARG:C  | 1:325:A:GLN:N | 2                   | 7.53  | 2.41            | 7.53   |
| (1,133) | 1:375:A:ALA:C | 1:376:A:GLN:N  | 1:376:A:GLN:CA | 1:376:A:GLN:C | 2                   | 7.5   | 1.88            | 7.5    |
| (1,256) | 1:478:A:TRP:C | 1:479:A:ASN:N  | 1:479:A:ASN:CA | 1:479:A:ASN:C | 2                   | 5.54  | 2.1             | 5.54   |
| (1,117) | 1:361:A:LEU:C | 1:362:A:HIS:N  | 1:362:A:HIS:CA | 1:362:A:HIS:C | 2                   | 4.96  | 2.12            | 4.96   |
| (1,261) | 1:481:A:SER:N | 1:481:A:SER:CA | 1:481:A:SER:C  | 1:482:A:THR:N | 2                   | 4.82  | 3.5             | 4.82   |
| (1,58)  | 1:319:A:ASN:N | 1:319:A:ASN:CA | 1:319:A:ASN:C  | 1:320:A:ASP:N | 2                   | 4.32  | 2.84            | 4.32   |
| (1,126) | 1:366:A:MET:N | 1:366:A:MET:CA | 1:366:A:MET:C  | 1:367:A:VAL:N | 2                   | 4.08  | 0.89            | 4.08   |
| (1,233) | 1:461:A:VAL:C | 1:462:A:GLY:N  | 1:462:A:GLY:CA | 1:462:A:GLY:C | 2                   | 2.94  | 0.49            | 2.94   |
| (1,129) | 1:372:A:ASN:C | 1:373:A:SER:N  | 1:373:A:SER:CA | 1:373:A:SER:C | 2                   | 2.31  | 0.27            | 2.31   |
| (1,209) | 1:444:A:GLY:C | 1:445:A:GLN:N  | 1:445:A:GLN:CA | 1:445:A:GLN:C | 2                   | 1.61  | 0.4             | 1.61   |
| (1,276) | 1:491:A:THR:C | 1:492:A:ILE:N  | 1:492:A:ILE:CA | 1:492:A:ILE:C | 2                   | 1.42  | 0.39            | 1.42   |

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

## 10.5 All violated dihedral-angle restraints ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,112) | 1:353:A:THR:N | 1:353:A:THR:CA | 1:353:A:THR:C  | 1:354:A:GLY:N | 6        | 127.09        |
| (1,110) | 1:350:A:SER:N | 1:350:A:SER:CA | 1:350:A:SER:C  | 1:351:A:GLY:N | 8        | 81.39         |
| (1,112) | 1:353:A:THR:N | 1:353:A:THR:CA | 1:353:A:THR:C  | 1:354:A:GLY:N | 1        | 73.38         |
| (1,112) | 1:353:A:THR:N | 1:353:A:THR:CA | 1:353:A:THR:C  | 1:354:A:GLY:N | 8        | 59.53         |
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 3        | 57.72         |
| (1,112) | 1:353:A:THR:N | 1:353:A:THR:CA | 1:353:A:THR:C  | 1:354:A:GLY:N | 7        | 50.36         |
| (1,111) | 1:352:A:SER:C | 1:353:A:THR:N  | 1:353:A:THR:CA | 1:353:A:THR:C | 13       | 48.46         |
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 5        | 43.81         |
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 2        | 42.3          |
| (1,127) | 1:370:A:PHE:C | 1:371:A:SER:N  | 1:371:A:SER:CA | 1:371:A:SER:C | 12       | 42.29         |
| (1,113) | 1:356:A:SER:C | 1:357:A:THR:N  | 1:357:A:THR:CA | 1:357:A:THR:C | 12       | 41.52         |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 13       | 39.56         |
| (1,127) | 1:370:A:PHE:C | 1:371:A:SER:N  | 1:371:A:SER:CA | 1:371:A:SER:C | 7        | 37.82         |
| (1,127) | 1:370:A:PHE:C | 1:371:A:SER:N  | 1:371:A:SER:CA | 1:371:A:SER:C | 3        | 36.45         |
| (1,2)   | 1:259:A:ASN:N | 1:259:A:ASN:CA | 1:259:A:ASN:C  | 1:260:A:ASN:N | 14       | 35.66         |
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 14       | 35.43         |
| (1,127) | 1:370:A:PHE:C | 1:371:A:SER:N  | 1:371:A:SER:CA | 1:371:A:SER:C | 1        | 35.24         |
| (1,111) | 1:352:A:SER:C | 1:353:A:THR:N  | 1:353:A:THR:CA | 1:353:A:THR:C | 2        | 34.83         |
| (1,115) | 1:360:A:HIS:C | 1:361:A:LEU:N  | 1:361:A:LEU:CA | 1:361:A:LEU:C | 5        | 32.86         |
| (1,111) | 1:352:A:SER:C | 1:353:A:THR:N  | 1:353:A:THR:CA | 1:353:A:THR:C | 5        | 32.39         |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 12       | 32.1          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 1        | 31.6          |
| (1,202) | 1:439:A:GLY:N | 1:439:A:GLY:CA | 1:439:A:GLY:C  | 1:440:A:VAL:N | 15       | 31.5          |
| (1,127) | 1:370:A:PHE:C | 1:371:A:SER:N  | 1:371:A:SER:CA | 1:371:A:SER:C | 2        | 31.39         |
| (1,115) | 1:360:A:HIS:C | 1:361:A:LEU:N  | 1:361:A:LEU:CA | 1:361:A:LEU:C | 3        | 30.16         |
| (1,127) | 1:370:A:PHE:C | 1:371:A:SER:N  | 1:371:A:SER:CA | 1:371:A:SER:C | 15       | 30.01         |
| (1,111) | 1:352:A:SER:C | 1:353:A:THR:N  | 1:353:A:THR:CA | 1:353:A:THR:C | 4        | 29.84         |
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 11       | 29.49         |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 1        | 29.1          |
| (1,113) | 1:356:A:SER:C | 1:357:A:THR:N  | 1:357:A:THR:CA | 1:357:A:THR:C | 9        | 29.06         |
| (1,127) | 1:370:A:PHE:C | 1:371:A:SER:N  | 1:371:A:SER:CA | 1:371:A:SER:C | 4        | 28.5          |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 10       | 28.3          |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 13       | 27.76         |
| (1,127) | 1:370:A:PHE:C | 1:371:A:SER:N  | 1:371:A:SER:CA | 1:371:A:SER:C | 11       | 27.72         |
| (1,115) | 1:360:A:HIS:C | 1:361:A:LEU:N  | 1:361:A:LEU:CA | 1:361:A:LEU:C | 12       | 27.71         |
| (1,127) | 1:370:A:PHE:C | 1:371:A:SER:N  | 1:371:A:SER:CA | 1:371:A:SER:C | 13       | 27.67         |
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 8        | 27.37         |
| (1,262) | 1:481:A:SER:C | 1:482:A:THR:N  | 1:482:A:THR:CA | 1:482:A:THR:C | 12       | 27.3          |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 9        | 27.02         |
| (1,115) | 1:360:A:HIS:C | 1:361:A:LEU:N  | 1:361:A:LEU:CA | 1:361:A:LEU:C | 11       | 26.92         |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 3        | 26.71         |
| (1,111) | 1:352:A:SER:C | 1:353:A:THR:N  | 1:353:A:THR:CA | 1:353:A:THR:C | 10       | 25.63         |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 8        | 25.27         |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 3        | 25.1          |
| (1,115) | 1:360:A:HIS:C | 1:361:A:LEU:N  | 1:361:A:LEU:CA | 1:361:A:LEU:C | 14       | 24.52         |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 3        | 24.21         |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 15       | 24.03         |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 5        | 23.92         |
| (1,262) | 1:481:A:SER:C | 1:482:A:THR:N  | 1:482:A:THR:CA | 1:482:A:THR:C | 5        | 23.43         |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 11       | 23.39         |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 9        | 22.93         |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 1        | 22.5          |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 15       | 22.33         |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 2        | 21.67         |
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 9        | 21.66         |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 15       | 21.43         |
| (1,115) | 1:360:A:HIS:C | 1:361:A:LEU:N  | 1:361:A:LEU:CA | 1:361:A:LEU:C | 10       | 21.34         |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 10       | 20.92         |
| (1,127) | 1:370:A:PHE:C | 1:371:A:SER:N  | 1:371:A:SER:CA | 1:371:A:SER:C | 5        | 20.86         |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 6        | 20.63         |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 6        | 20.56         |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 2        | 20.49         |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 2        | 20.15         |
| (1,113) | 1:356:A:SER:C | 1:357:A:THR:N  | 1:357:A:THR:CA | 1:357:A:THR:C | 4        | 20.15         |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 4        | 20.03         |
| (1,11)  | 1:277:A:GLY:C | 1:278:A:MET:N  | 1:278:A:MET:CA | 1:278:A:MET:C | 9        | 19.99         |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 5        | 19.95         |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 5        | 19.83         |
| (1,11)  | 1:277:A:GLY:C | 1:278:A:MET:N  | 1:278:A:MET:CA | 1:278:A:MET:C | 12       | 19.67         |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 2        | 19.02         |
| (1,45)  | 1:306:A:SER:C | 1:307:A:ASN:N  | 1:307:A:ASN:CA | 1:307:A:ASN:C | 11       | 19.0          |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 14       | 18.97         |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 4        | 18.68         |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 6        | 18.64         |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 11       | 18.64         |
| (1,59)  | 1:319:A:ASN:C | 1:320:A:ASP:N  | 1:320:A:ASP:CA | 1:320:A:ASP:C | 1        | 18.58         |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 9        | 18.57         |
| (1,91)  | 1:340:A:TYR:C | 1:341:A:VAL:N  | 1:341:A:VAL:CA | 1:341:A:VAL:C | 11       | 18.56         |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 11       | 18.5          |
| (1,114) | 1:357:A:THR:N | 1:357:A:THR:CA | 1:357:A:THR:C  | 1:358:A:ALA:N | 4        | 18.22         |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 2        | 18.18         |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 14       | 18.17         |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 10       | 17.95         |
| (1,62)  | 1:321:A:GLY:N | 1:321:A:GLY:CA | 1:321:A:GLY:C  | 1:322:A:VAL:N | 12       | 17.94         |
| (1,112) | 1:353:A:THR:N | 1:353:A:THR:CA | 1:353:A:THR:C  | 1:354:A:GLY:N | 14       | 17.93         |
| (1,59)  | 1:319:A:ASN:C | 1:320:A:ASP:N  | 1:320:A:ASP:CA | 1:320:A:ASP:C | 13       | 17.85         |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 12       | 17.8          |
| (1,127) | 1:370:A:PHE:C | 1:371:A:SER:N  | 1:371:A:SER:CA | 1:371:A:SER:C | 14       | 17.71         |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 8        | 17.67         |
| (1,262) | 1:481:A:SER:C | 1:482:A:THR:N  | 1:482:A:THR:CA | 1:482:A:THR:C | 14       | 17.54         |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 6        | 17.48         |
| (1,176) | 1:416:A:ALA:C | 1:417:A:SER:N  | 1:417:A:SER:CA | 1:417:A:SER:C | 10       | 17.45         |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 1        | 17.2          |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 15       | 17.2          |
| (1,262) | 1:481:A:SER:C | 1:482:A:THR:N  | 1:482:A:THR:CA | 1:482:A:THR:C | 3        | 17.06         |
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 4        | 17.01         |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 8        | 16.71         |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 10       | 16.6          |
| (1,112) | 1:353:A:THR:N | 1:353:A:THR:CA | 1:353:A:THR:C  | 1:354:A:GLY:N | 13       | 16.6          |
| (1,176) | 1:416:A:ALA:C | 1:417:A:SER:N  | 1:417:A:SER:CA | 1:417:A:SER:C | 15       | 16.58         |
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 13       | 16.56         |
| (1,77)  | 1:332:A:LYS:C | 1:333:A:TYR:N  | 1:333:A:TYR:CA | 1:333:A:TYR:C | 15       | 16.35         |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 11       | 16.33         |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 14       | 16.3          |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 12       | 16.25         |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 8        | 16.12         |
| (1,111) | 1:352:A:SER:C | 1:353:A:THR:N  | 1:353:A:THR:CA | 1:353:A:THR:C | 9        | 16.05         |
| (1,111) | 1:352:A:SER:C | 1:353:A:THR:N  | 1:353:A:THR:CA | 1:353:A:THR:C | 3        | 15.91         |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 6        | 15.72         |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 3        | 15.71         |
| (1,262) | 1:481:A:SER:C | 1:482:A:THR:N  | 1:482:A:THR:CA | 1:482:A:THR:C | 7        | 15.64         |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 13       | 15.58         |
| (1,33)  | 1:295:A:ILE:C | 1:296:A:SER:N  | 1:296:A:SER:CA | 1:296:A:SER:C | 15       | 15.37         |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 15       | 15.22         |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 1        | 15.02         |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 11       | 14.87         |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 6        | 14.58         |
| (1,37)  | 1:298:A:GLY:C | 1:299:A:LYS:N  | 1:299:A:LYS:CA | 1:299:A:LYS:C | 11       | 14.4          |
| (1,176) | 1:416:A:ALA:C | 1:417:A:SER:N  | 1:417:A:SER:CA | 1:417:A:SER:C | 9        | 14.39         |
| (1,263) | 1:482:A:THR:N | 1:482:A:THR:CA | 1:482:A:THR:C  | 1:483:A:ASN:N | 9        | 14.38         |
| (1,155) | 1:402:A:TRP:N | 1:402:A:TRP:CA | 1:402:A:TRP:C  | 1:403:A:LYS:N | 7        | 14.34         |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 12       | 14.32         |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 4        | 14.26         |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,11)  | 1:277:A:GLY:C | 1:278:A:MET:N  | 1:278:A:MET:CA | 1:278:A:MET:C | 2        | 14.21         |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 10       | 14.19         |
| (1,176) | 1:416:A:ALA:C | 1:417:A:SER:N  | 1:417:A:SER:CA | 1:417:A:SER:C | 12       | 14.12         |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 7        | 13.82         |
| (1,37)  | 1:298:A:GLY:C | 1:299:A:LYS:N  | 1:299:A:LYS:CA | 1:299:A:LYS:C | 9        | 13.71         |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 8        | 13.69         |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 3        | 13.68         |
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 6        | 13.62         |
| (1,16)  | 1:280:A:TYR:N | 1:280:A:TYR:CA | 1:280:A:TYR:C  | 1:281:A:GLY:N | 7        | 13.28         |
| (1,277) | 1:492:A:ILE:N | 1:492:A:ILE:CA | 1:492:A:ILE:C  | 1:493:A:LYS:N | 10       | 13.22         |
| (1,37)  | 1:298:A:GLY:C | 1:299:A:LYS:N  | 1:299:A:LYS:CA | 1:299:A:LYS:C | 1        | 13.18         |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 13       | 13.04         |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 7        | 12.92         |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 2        | 12.92         |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 13       | 12.9          |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 1        | 12.7          |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 3        | 12.69         |
| (1,62)  | 1:321:A:GLY:N | 1:321:A:GLY:CA | 1:321:A:GLY:C  | 1:322:A:VAL:N | 3        | 12.66         |
| (1,11)  | 1:277:A:GLY:C | 1:278:A:MET:N  | 1:278:A:MET:CA | 1:278:A:MET:C | 4        | 12.54         |
| (1,90)  | 1:340:A:TYR:N | 1:340:A:TYR:CA | 1:340:A:TYR:C  | 1:341:A:VAL:N | 11       | 12.39         |
| (1,15)  | 1:279:A:HIS:C | 1:280:A:TYR:N  | 1:280:A:TYR:CA | 1:280:A:TYR:C | 14       | 12.39         |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 8        | 12.29         |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 5        | 12.22         |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 8        | 12.2          |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 4        | 12.13         |
| (1,17)  | 1:280:A:TYR:C | 1:281:A:GLY:N  | 1:281:A:GLY:CA | 1:281:A:GLY:C | 11       | 12.11         |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 15       | 11.94         |
| (1,254) | 1:477:A:THR:C | 1:478:A:TRP:N  | 1:478:A:TRP:CA | 1:478:A:TRP:C | 12       | 11.91         |
| (1,198) | 1:433:A:ARG:N | 1:433:A:ARG:CA | 1:433:A:ARG:C  | 1:434:A:SER:N | 13       | 11.82         |
| (1,262) | 1:481:A:SER:C | 1:482:A:THR:N  | 1:482:A:THR:CA | 1:482:A:THR:C | 8        | 11.8          |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 10       | 11.77         |
| (1,155) | 1:402:A:TRP:N | 1:402:A:TRP:CA | 1:402:A:TRP:C  | 1:403:A:LYS:N | 12       | 11.72         |
| (1,33)  | 1:295:A:ILE:C | 1:296:A:SER:N  | 1:296:A:SER:CA | 1:296:A:SER:C | 1        | 11.47         |
| (1,254) | 1:477:A:THR:C | 1:478:A:TRP:N  | 1:478:A:TRP:CA | 1:478:A:TRP:C | 6        | 11.38         |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 1        | 11.38         |
| (1,115) | 1:360:A:HIS:C | 1:361:A:LEU:N  | 1:361:A:LEU:CA | 1:361:A:LEU:C | 15       | 11.38         |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 7        | 11.33         |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 1        | 11.27         |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 6        | 11.24         |
| (1,176) | 1:416:A:ALA:C | 1:417:A:SER:N  | 1:417:A:SER:CA | 1:417:A:SER:C | 2        | 11.19         |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 14       | 11.12         |
| (1,12)  | 1:278:A:MET:N | 1:278:A:MET:CA | 1:278:A:MET:C  | 1:279:A:HIS:N | 1        | 11.12         |
| (1,62)  | 1:321:A:GLY:N | 1:321:A:GLY:CA | 1:321:A:GLY:C  | 1:322:A:VAL:N | 14       | 11.0          |
| (1,15)  | 1:279:A:HIS:C | 1:280:A:TYR:N  | 1:280:A:TYR:CA | 1:280:A:TYR:C | 15       | 10.83         |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 14       | 10.82         |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 2        | 10.76         |
| (1,273) | 1:490:A:GLY:N | 1:490:A:GLY:CA | 1:490:A:GLY:C  | 1:491:A:THR:N | 1        | 10.75         |
| (1,254) | 1:477:A:THR:C | 1:478:A:TRP:N  | 1:478:A:TRP:CA | 1:478:A:TRP:C | 7        | 10.52         |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 13       | 10.51         |
| (1,202) | 1:439:A:GLY:N | 1:439:A:GLY:CA | 1:439:A:GLY:C  | 1:440:A:VAL:N | 13       | 10.5          |
| (1,77)  | 1:332:A:LYS:C | 1:333:A:TYR:N  | 1:333:A:TYR:CA | 1:333:A:TYR:C | 1        | 10.47         |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 14       | 10.43         |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 9        | 10.4          |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 3        | 10.21         |
| (1,155) | 1:402:A:TRP:N | 1:402:A:TRP:CA | 1:402:A:TRP:C  | 1:403:A:LYS:N | 6        | 10.18         |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 11       | 10.13         |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 5        | 10.05         |
| (1,262) | 1:481:A:SER:C | 1:482:A:THR:N  | 1:482:A:THR:CA | 1:482:A:THR:C | 11       | 10.03         |
| (1,64)  | 1:324:A:ARG:N | 1:324:A:ARG:CA | 1:324:A:ARG:C  | 1:325:A:GLN:N | 11       | 9.94          |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 10       | 9.81          |
| (1,202) | 1:439:A:GLY:N | 1:439:A:GLY:CA | 1:439:A:GLY:C  | 1:440:A:VAL:N | 3        | 9.8           |
| (1,155) | 1:402:A:TRP:N | 1:402:A:TRP:CA | 1:402:A:TRP:C  | 1:403:A:LYS:N | 3        | 9.77          |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 3        | 9.7           |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 4        | 9.66          |
| (1,63)  | 1:323:A:HIS:C | 1:324:A:ARG:N  | 1:324:A:ARG:CA | 1:324:A:ARG:C | 7        | 9.61          |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 15       | 9.6           |
| (1,198) | 1:433:A:ARG:N | 1:433:A:ARG:CA | 1:433:A:ARG:C  | 1:434:A:SER:N | 5        | 9.52          |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 11       | 9.47          |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 14       | 9.44          |
| (1,273) | 1:490:A:GLY:N | 1:490:A:GLY:CA | 1:490:A:GLY:C  | 1:491:A:THR:N | 3        | 9.38          |
| (1,133) | 1:375:A:ALA:C | 1:376:A:GLN:N  | 1:376:A:GLN:CA | 1:376:A:GLN:C | 8        | 9.38          |
| (1,176) | 1:416:A:ALA:C | 1:417:A:SER:N  | 1:417:A:SER:CA | 1:417:A:SER:C | 7        | 9.37          |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 10       | 9.37          |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 13       | 9.35          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 2        | 9.34          |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 14       | 9.26          |
| (1,202) | 1:439:A:GLY:N | 1:439:A:GLY:CA | 1:439:A:GLY:C  | 1:440:A:VAL:N | 9        | 9.18          |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 7        | 9.03          |
| (1,77)  | 1:332:A:LYS:C | 1:333:A:TYR:N  | 1:333:A:TYR:CA | 1:333:A:TYR:C | 13       | 8.85          |
| (1,18)  | 1:281:A:GLY:N | 1:281:A:GLY:CA | 1:281:A:GLY:C  | 1:282:A:VAL:N | 3        | 8.74          |
| (1,176) | 1:416:A:ALA:C | 1:417:A:SER:N  | 1:417:A:SER:CA | 1:417:A:SER:C | 4        | 8.65          |
| (1,176) | 1:416:A:ALA:C | 1:417:A:SER:N  | 1:417:A:SER:CA | 1:417:A:SER:C | 14       | 8.62          |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 7        | 8.58          |
| (1,273) | 1:490:A:GLY:N | 1:490:A:GLY:CA | 1:490:A:GLY:C  | 1:491:A:THR:N | 7        | 8.55          |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 12       | 8.46          |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 9        | 8.41          |
| (1,262) | 1:481:A:SER:C | 1:482:A:THR:N  | 1:482:A:THR:CA | 1:482:A:THR:C | 15       | 8.39          |
| (1,155) | 1:402:A:TRP:N | 1:402:A:TRP:CA | 1:402:A:TRP:C  | 1:403:A:LYS:N | 9        | 8.39          |
| (1,155) | 1:402:A:TRP:N | 1:402:A:TRP:CA | 1:402:A:TRP:C  | 1:403:A:LYS:N | 4        | 8.37          |
| (1,33)  | 1:295:A:ILE:C | 1:296:A:SER:N  | 1:296:A:SER:CA | 1:296:A:SER:C | 4        | 8.34          |
| (1,261) | 1:481:A:SER:N | 1:481:A:SER:CA | 1:481:A:SER:C  | 1:482:A:THR:N | 12       | 8.33          |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 15       | 8.32          |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 9        | 8.29          |
| (1,33)  | 1:295:A:ILE:C | 1:296:A:SER:N  | 1:296:A:SER:CA | 1:296:A:SER:C | 8        | 8.29          |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 4        | 8.27          |
| (1,202) | 1:439:A:GLY:N | 1:439:A:GLY:CA | 1:439:A:GLY:C  | 1:440:A:VAL:N | 2        | 8.27          |
| (1,198) | 1:433:A:ARG:N | 1:433:A:ARG:CA | 1:433:A:ARG:C  | 1:434:A:SER:N | 9        | 8.23          |
| (1,11)  | 1:277:A:GLY:C | 1:278:A:MET:N  | 1:278:A:MET:CA | 1:278:A:MET:C | 14       | 8.22          |
| (1,202) | 1:439:A:GLY:N | 1:439:A:GLY:CA | 1:439:A:GLY:C  | 1:440:A:VAL:N | 14       | 8.18          |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 4        | 8.18          |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 7        | 8.17          |
| (1,135) | 1:376:A:GLN:C | 1:377:A:ASP:N  | 1:377:A:ASP:CA | 1:377:A:ASP:C | 7        | 8.09          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 5        | 8.07          |
| (1,18)  | 1:281:A:GLY:N | 1:281:A:GLY:CA | 1:281:A:GLY:C  | 1:282:A:VAL:N | 12       | 7.98          |
| (1,273) | 1:490:A:GLY:N | 1:490:A:GLY:CA | 1:490:A:GLY:C  | 1:491:A:THR:N | 11       | 7.96          |
| (1,18)  | 1:281:A:GLY:N | 1:281:A:GLY:CA | 1:281:A:GLY:C  | 1:282:A:VAL:N | 10       | 7.96          |
| (1,262) | 1:481:A:SER:C | 1:482:A:THR:N  | 1:482:A:THR:CA | 1:482:A:THR:C | 13       | 7.92          |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 8        | 7.87          |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 2        | 7.85          |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 2        | 7.85          |
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 15       | 7.82          |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 9        | 7.8           |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 14       | 7.78          |
| (1,15)  | 1:279:A:HIS:C | 1:280:A:TYR:N  | 1:280:A:TYR:CA | 1:280:A:TYR:C | 2        | 7.76          |
| (1,11)  | 1:277:A:GLY:C | 1:278:A:MET:N  | 1:278:A:MET:CA | 1:278:A:MET:C | 6        | 7.73          |
| (1,254) | 1:477:A:THR:C | 1:478:A:TRP:N  | 1:478:A:TRP:CA | 1:478:A:TRP:C | 8        | 7.71          |
| (1,256) | 1:478:A:TRP:C | 1:479:A:ASN:N  | 1:479:A:ASN:CA | 1:479:A:ASN:C | 2        | 7.63          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 13       | 7.61          |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 1        | 7.61          |
| (1,11)  | 1:277:A:GLY:C | 1:278:A:MET:N  | 1:278:A:MET:CA | 1:278:A:MET:C | 8        | 7.55          |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 11       | 7.5           |
| (1,62)  | 1:321:A:GLY:N | 1:321:A:GLY:CA | 1:321:A:GLY:C  | 1:322:A:VAL:N | 7        | 7.47          |
| (1,262) | 1:481:A:SER:C | 1:482:A:THR:N  | 1:482:A:THR:CA | 1:482:A:THR:C | 9        | 7.45          |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 6        | 7.33          |
| (1,254) | 1:477:A:THR:C | 1:478:A:TRP:N  | 1:478:A:TRP:CA | 1:478:A:TRP:C | 3        | 7.3           |
| (1,18)  | 1:281:A:GLY:N | 1:281:A:GLY:CA | 1:281:A:GLY:C  | 1:282:A:VAL:N | 5        | 7.28          |
| (1,254) | 1:477:A:THR:C | 1:478:A:TRP:N  | 1:478:A:TRP:CA | 1:478:A:TRP:C | 13       | 7.27          |
| (1,263) | 1:482:A:THR:N | 1:482:A:THR:CA | 1:482:A:THR:C  | 1:483:A:ASN:N | 14       | 7.25          |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 4        | 7.19          |
| (1,155) | 1:402:A:TRP:N | 1:402:A:TRP:CA | 1:402:A:TRP:C  | 1:403:A:LYS:N | 1        | 7.16          |
| (1,58)  | 1:319:A:ASN:N | 1:319:A:ASN:CA | 1:319:A:ASN:C  | 1:320:A:ASP:N | 13       | 7.16          |
| (1,37)  | 1:298:A:GLY:C | 1:299:A:LYS:N  | 1:299:A:LYS:CA | 1:299:A:LYS:C | 10       | 7.14          |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 12       | 7.13          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 12       | 7.12          |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 7        | 7.09          |
| (1,117) | 1:361:A:LEU:C | 1:362:A:HIS:N  | 1:362:A:HIS:CA | 1:362:A:HIS:C | 3        | 7.08          |
| (1,262) | 1:481:A:SER:C | 1:482:A:THR:N  | 1:482:A:THR:CA | 1:482:A:THR:C | 4        | 7.06          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 7        | 6.9           |
| (1,254) | 1:477:A:THR:C | 1:478:A:TRP:N  | 1:478:A:TRP:CA | 1:478:A:TRP:C | 9        | 6.88          |
| (1,202) | 1:439:A:GLY:N | 1:439:A:GLY:CA | 1:439:A:GLY:C  | 1:440:A:VAL:N | 1        | 6.87          |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 11       | 6.87          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 11       | 6.79          |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 3        | 6.77          |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 2        | 6.76          |
| (1,18)  | 1:281:A:GLY:N | 1:281:A:GLY:CA | 1:281:A:GLY:C  | 1:282:A:VAL:N | 1        | 6.75          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 15       | 6.69          |
| (1,33)  | 1:295:A:ILE:C | 1:296:A:SER:N  | 1:296:A:SER:CA | 1:296:A:SER:C | 6        | 6.69          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 10       | 6.67          |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 7        | 6.66          |
| (1,47)  | 1:312:A:ASN:C | 1:313:A:GLN:N  | 1:313:A:GLN:CA | 1:313:A:GLN:C | 2        | 6.62          |
| (1,202) | 1:439:A:GLY:N | 1:439:A:GLY:CA | 1:439:A:GLY:C  | 1:440:A:VAL:N | 6        | 6.61          |
| (1,262) | 1:481:A:SER:C | 1:482:A:THR:N  | 1:482:A:THR:CA | 1:482:A:THR:C | 1        | 6.57          |
| (1,154) | 1:401:A:GLY:C | 1:402:A:TRP:N  | 1:402:A:TRP:CA | 1:402:A:TRP:C | 15       | 6.56          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 9        | 6.53          |
| (1,15)  | 1:279:A:HIS:C | 1:280:A:TYR:N  | 1:280:A:TYR:CA | 1:280:A:TYR:C | 8        | 6.52          |
| (1,196) | 1:432:A:PHE:N | 1:432:A:PHE:CA | 1:432:A:PHE:C  | 1:433:A:ARG:N | 1        | 6.39          |
| (1,254) | 1:477:A:THR:C | 1:478:A:TRP:N  | 1:478:A:TRP:CA | 1:478:A:TRP:C | 4        | 6.33          |
| (1,226) | 1:455:A:GLN:N | 1:455:A:GLN:CA | 1:455:A:GLN:C  | 1:456:A:ASP:N | 7        | 6.24          |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 5        | 6.24          |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 10       | 6.2           |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 8        | 6.19          |
| (1,33)  | 1:295:A:ILE:C | 1:296:A:SER:N  | 1:296:A:SER:CA | 1:296:A:SER:C | 13       | 6.18          |
| (1,263) | 1:482:A:THR:N | 1:482:A:THR:CA | 1:482:A:THR:C  | 1:483:A:ASN:N | 3        | 6.16          |
| (1,258) | 1:479:A:ASN:C | 1:480:A:LYS:N  | 1:480:A:LYS:CA | 1:480:A:LYS:C | 11       | 6.15          |
| (1,21)  | 1:282:A:VAL:C | 1:283:A:ASP:N  | 1:283:A:ASP:CA | 1:283:A:ASP:C | 15       | 5.97          |
| (1,154) | 1:401:A:GLY:C | 1:402:A:TRP:N  | 1:402:A:TRP:CA | 1:402:A:TRP:C | 8        | 5.95          |
| (1,254) | 1:477:A:THR:C | 1:478:A:TRP:N  | 1:478:A:TRP:CA | 1:478:A:TRP:C | 10       | 5.91          |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 12       | 5.86          |
| (1,273) | 1:490:A:GLY:N | 1:490:A:GLY:CA | 1:490:A:GLY:C  | 1:491:A:THR:N | 14       | 5.82          |
| (1,18)  | 1:281:A:GLY:N | 1:281:A:GLY:CA | 1:281:A:GLY:C  | 1:282:A:VAL:N | 14       | 5.81          |
| (1,263) | 1:482:A:THR:N | 1:482:A:THR:CA | 1:482:A:THR:C  | 1:483:A:ASN:N | 7        | 5.76          |
| (1,198) | 1:433:A:ARG:N | 1:433:A:ARG:CA | 1:433:A:ARG:C  | 1:434:A:SER:N | 12       | 5.73          |
| (1,254) | 1:477:A:THR:C | 1:478:A:TRP:N  | 1:478:A:TRP:CA | 1:478:A:TRP:C | 2        | 5.68          |
| (1,133) | 1:375:A:ALA:C | 1:376:A:GLN:N  | 1:376:A:GLN:CA | 1:376:A:GLN:C | 5        | 5.62          |
| (1,151) | 1:386:A:GLY:N | 1:386:A:GLY:CA | 1:386:A:GLY:C  | 1:387:A:TYR:N | 15       | 5.58          |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 7        | 5.57          |
| (1,151) | 1:386:A:GLY:N | 1:386:A:GLY:CA | 1:386:A:GLY:C  | 1:387:A:TYR:N | 2        | 5.55          |
| (1,151) | 1:386:A:GLY:N | 1:386:A:GLY:CA | 1:386:A:GLY:C  | 1:387:A:TYR:N | 12       | 5.55          |
| (1,77)  | 1:332:A:LYS:C | 1:333:A:TYR:N  | 1:333:A:TYR:CA | 1:333:A:TYR:C | 6        | 5.52          |
| (1,210) | 1:445:A:GLN:N | 1:445:A:GLN:CA | 1:445:A:GLN:C  | 1:446:A:THR:N | 8        | 5.48          |
| (1,15)  | 1:279:A:HIS:C | 1:280:A:TYR:N  | 1:280:A:TYR:CA | 1:280:A:TYR:C | 3        | 5.46          |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 13       | 5.44          |
| (1,33)  | 1:295:A:ILE:C | 1:296:A:SER:N  | 1:296:A:SER:CA | 1:296:A:SER:C | 9        | 5.4           |
| (1,215) | 1:448:A:HIS:C | 1:449:A:TYR:N  | 1:449:A:TYR:CA | 1:449:A:TYR:C | 5        | 5.38          |
| (1,150) | 1:385:A:ALA:C | 1:386:A:GLY:N  | 1:386:A:GLY:CA | 1:386:A:GLY:C | 9        | 5.38          |
| (1,154) | 1:401:A:GLY:C | 1:402:A:TRP:N  | 1:402:A:TRP:CA | 1:402:A:TRP:C | 5        | 5.36          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 4        | 5.27          |
| (1,273) | 1:490:A:GLY:N | 1:490:A:GLY:CA | 1:490:A:GLY:C  | 1:491:A:THR:N | 5        | 5.24          |
| (1,273) | 1:490:A:GLY:N | 1:490:A:GLY:CA | 1:490:A:GLY:C  | 1:491:A:THR:N | 13       | 5.24          |
| (1,198) | 1:433:A:ARG:N | 1:433:A:ARG:CA | 1:433:A:ARG:C  | 1:434:A:SER:N | 3        | 5.22          |
| (1,119) | 1:362:A:HIS:C | 1:363:A:PHE:N  | 1:363:A:PHE:CA | 1:363:A:PHE:C | 15       | 5.21          |
| (1,77)  | 1:332:A:LYS:C | 1:333:A:TYR:N  | 1:333:A:TYR:CA | 1:333:A:TYR:C | 12       | 5.17          |
| (1,198) | 1:433:A:ARG:N | 1:433:A:ARG:CA | 1:433:A:ARG:C  | 1:434:A:SER:N | 11       | 5.13          |
| (1,64)  | 1:324:A:ARG:N | 1:324:A:ARG:CA | 1:324:A:ARG:C  | 1:325:A:GLN:N | 14       | 5.12          |
| (1,62)  | 1:321:A:GLY:N | 1:321:A:GLY:CA | 1:321:A:GLY:C  | 1:322:A:VAL:N | 6        | 5.05          |
| (1,273) | 1:490:A:GLY:N | 1:490:A:GLY:CA | 1:490:A:GLY:C  | 1:491:A:THR:N | 2        | 5.04          |
| (1,202) | 1:439:A:GLY:N | 1:439:A:GLY:CA | 1:439:A:GLY:C  | 1:440:A:VAL:N | 10       | 5.04          |
| (1,18)  | 1:281:A:GLY:N | 1:281:A:GLY:CA | 1:281:A:GLY:C  | 1:282:A:VAL:N | 9        | 5.01          |
| (1,17)  | 1:280:A:TYR:C | 1:281:A:GLY:N  | 1:281:A:GLY:CA | 1:281:A:GLY:C | 2        | 5.01          |
| (1,126) | 1:366:A:MET:N | 1:366:A:MET:CA | 1:366:A:MET:C  | 1:367:A:VAL:N | 8        | 4.97          |
| (1,4)   | 1:263:A:LYS:N | 1:263:A:LYS:CA | 1:263:A:LYS:C  | 1:264:A:GLY:N | 5        | 4.84          |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 1        | 4.8           |
| (1,202) | 1:439:A:GLY:N | 1:439:A:GLY:CA | 1:439:A:GLY:C  | 1:440:A:VAL:N | 4        | 4.78          |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 5        | 4.74          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,187) | 1:423:A:ASP:C | 1:424:A:ILE:N  | 1:424:A:ILE:CA | 1:424:A:ILE:C | 11       | 4.73          |
| (1,135) | 1:376:A:GLN:C | 1:377:A:ASP:N  | 1:377:A:ASP:CA | 1:377:A:ASP:C | 4        | 4.65          |
| (1,187) | 1:423:A:ASP:C | 1:424:A:ILE:N  | 1:424:A:ILE:CA | 1:424:A:ILE:C | 9        | 4.63          |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 4        | 4.61          |
| (1,33)  | 1:295:A:ILE:C | 1:296:A:SER:N  | 1:296:A:SER:CA | 1:296:A:SER:C | 11       | 4.6           |
| (1,17)  | 1:280:A:TYR:C | 1:281:A:GLY:N  | 1:281:A:GLY:CA | 1:281:A:GLY:C | 14       | 4.5           |
| (1,198) | 1:433:A:ARG:N | 1:433:A:ARG:CA | 1:433:A:ARG:C  | 1:434:A:SER:N | 8        | 4.43          |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 3        | 4.41          |
| (1,155) | 1:402:A:TRP:N | 1:402:A:TRP:CA | 1:402:A:TRP:C  | 1:403:A:LYS:N | 14       | 4.32          |
| (1,254) | 1:477:A:THR:C | 1:478:A:TRP:N  | 1:478:A:TRP:CA | 1:478:A:TRP:C | 11       | 4.31          |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 6        | 4.3           |
| (1,135) | 1:376:A:GLN:C | 1:377:A:ASP:N  | 1:377:A:ASP:CA | 1:377:A:ASP:C | 12       | 4.27          |
| (1,15)  | 1:279:A:HIS:C | 1:280:A:TYR:N  | 1:280:A:TYR:CA | 1:280:A:TYR:C | 1        | 4.25          |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 15       | 4.24          |
| (1,72)  | 1:329:A:HIS:N | 1:329:A:HIS:CA | 1:329:A:HIS:C  | 1:330:A:LEU:N | 15       | 4.22          |
| (1,111) | 1:352:A:SER:C | 1:353:A:THR:N  | 1:353:A:THR:CA | 1:353:A:THR:C | 6        | 4.16          |
| (1,37)  | 1:298:A:GLY:C | 1:299:A:LYS:N  | 1:299:A:LYS:CA | 1:299:A:LYS:C | 15       | 4.16          |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 6        | 4.12          |
| (1,175) | 1:415:A:SER:N | 1:415:A:SER:CA | 1:415:A:SER:C  | 1:416:A:ALA:N | 1        | 4.1           |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 4        | 4.09          |
| (1,198) | 1:433:A:ARG:N | 1:433:A:ARG:CA | 1:433:A:ARG:C  | 1:434:A:SER:N | 1        | 4.06          |
| (1,111) | 1:352:A:SER:C | 1:353:A:THR:N  | 1:353:A:THR:CA | 1:353:A:THR:C | 8        | 4.02          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 1        | 3.99          |
| (1,33)  | 1:295:A:ILE:C | 1:296:A:SER:N  | 1:296:A:SER:CA | 1:296:A:SER:C | 2        | 3.94          |
| (1,15)  | 1:279:A:HIS:C | 1:280:A:TYR:N  | 1:280:A:TYR:CA | 1:280:A:TYR:C | 9        | 3.76          |
| (1,204) | 1:440:A:VAL:N | 1:440:A:VAL:CA | 1:440:A:VAL:C  | 1:441:A:LEU:N | 15       | 3.75          |
| (1,62)  | 1:321:A:GLY:N | 1:321:A:GLY:CA | 1:321:A:GLY:C  | 1:322:A:VAL:N | 1        | 3.7           |
| (1,273) | 1:490:A:GLY:N | 1:490:A:GLY:CA | 1:490:A:GLY:C  | 1:491:A:THR:N | 6        | 3.6           |
| (1,277) | 1:492:A:ILE:N | 1:492:A:ILE:CA | 1:492:A:ILE:C  | 1:493:A:LYS:N | 8        | 3.54          |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 14       | 3.53          |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 12       | 3.52          |
| (1,2)   | 1:259:A:ASN:N | 1:259:A:ASN:CA | 1:259:A:ASN:C  | 1:260:A:ASN:N | 9        | 3.51          |
| (1,59)  | 1:319:A:ASN:C | 1:320:A:ASP:N  | 1:320:A:ASP:CA | 1:320:A:ASP:C | 11       | 3.47          |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 3        | 3.47          |
| (1,256) | 1:478:A:TRP:C | 1:479:A:ASN:N  | 1:479:A:ASN:CA | 1:479:A:ASN:C | 12       | 3.44          |
| (1,233) | 1:461:A:VAL:C | 1:462:A:GLY:N  | 1:462:A:GLY:CA | 1:462:A:GLY:C | 8        | 3.43          |
| (1,11)  | 1:277:A:GLY:C | 1:278:A:MET:N  | 1:278:A:MET:CA | 1:278:A:MET:C | 1        | 3.38          |
| (1,196) | 1:432:A:PHE:N | 1:432:A:PHE:CA | 1:432:A:PHE:C  | 1:433:A:ARG:N | 5        | 3.37          |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 12       | 3.34          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 3        | 3.27          |
| (1,17)  | 1:280:A:TYR:C | 1:281:A:GLY:N  | 1:281:A:GLY:CA | 1:281:A:GLY:C | 15       | 3.22          |
| (1,273) | 1:490:A:GLY:N | 1:490:A:GLY:CA | 1:490:A:GLY:C  | 1:491:A:THR:N | 8        | 3.21          |
| (1,126) | 1:366:A:MET:N | 1:366:A:MET:CA | 1:366:A:MET:C  | 1:367:A:VAL:N | 5        | 3.19          |
| (1,176) | 1:416:A:ALA:C | 1:417:A:SER:N  | 1:417:A:SER:CA | 1:417:A:SER:C | 13       | 3.17          |
| (1,21)  | 1:282:A:VAL:C | 1:283:A:ASP:N  | 1:283:A:ASP:CA | 1:283:A:ASP:C | 11       | 3.17          |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 2        | 3.12          |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 15       | 3.1           |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 1        | 3.01          |
| (1,196) | 1:432:A:PHE:N | 1:432:A:PHE:CA | 1:432:A:PHE:C  | 1:433:A:ARG:N | 12       | 2.99          |
| (1,196) | 1:432:A:PHE:N | 1:432:A:PHE:CA | 1:432:A:PHE:C  | 1:433:A:ARG:N | 8        | 2.98          |
| (1,59)  | 1:319:A:ASN:C | 1:320:A:ASP:N  | 1:320:A:ASP:CA | 1:320:A:ASP:C | 3        | 2.98          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,247) | 1:472:A:TYR:C | 1:473:A:LEU:N  | 1:473:A:LEU:CA | 1:473:A:LEU:C | 3        | 2.96          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 14       | 2.92          |
| (1,33)  | 1:295:A:ILE:C | 1:296:A:SER:N  | 1:296:A:SER:CA | 1:296:A:SER:C | 14       | 2.86          |
| (1,117) | 1:361:A:LEU:C | 1:362:A:HIS:N  | 1:362:A:HIS:CA | 1:362:A:HIS:C | 12       | 2.85          |
| (1,18)  | 1:281:A:GLY:N | 1:281:A:GLY:CA | 1:281:A:GLY:C  | 1:282:A:VAL:N | 4        | 2.81          |
| (1,127) | 1:370:A:PHE:C | 1:371:A:SER:N  | 1:371:A:SER:CA | 1:371:A:SER:C | 8        | 2.8           |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 4        | 2.8           |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 11       | 2.76          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 6        | 2.69          |
| (1,18)  | 1:281:A:GLY:N | 1:281:A:GLY:CA | 1:281:A:GLY:C  | 1:282:A:VAL:N | 7        | 2.66          |
| (1,202) | 1:439:A:GLY:N | 1:439:A:GLY:CA | 1:439:A:GLY:C  | 1:440:A:VAL:N | 11       | 2.65          |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 5        | 2.62          |
| (1,21)  | 1:282:A:VAL:C | 1:283:A:ASP:N  | 1:283:A:ASP:CA | 1:283:A:ASP:C | 9        | 2.61          |
| (1,129) | 1:372:A:ASN:C | 1:373:A:SER:N  | 1:373:A:SER:CA | 1:373:A:SER:C | 5        | 2.58          |
| (1,85)  | 1:337:A:VAL:C | 1:338:A:GLY:N  | 1:338:A:GLY:CA | 1:338:A:GLY:C | 14       | 2.56          |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 14       | 2.55          |
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 10       | 2.54          |
| (1,62)  | 1:321:A:GLY:N | 1:321:A:GLY:CA | 1:321:A:GLY:C  | 1:322:A:VAL:N | 15       | 2.53          |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 13       | 2.49          |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 6        | 2.48          |
| (1,233) | 1:461:A:VAL:C | 1:462:A:GLY:N  | 1:462:A:GLY:CA | 1:462:A:GLY:C | 13       | 2.46          |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 13       | 2.46          |
| (1,273) | 1:490:A:GLY:N | 1:490:A:GLY:CA | 1:490:A:GLY:C  | 1:491:A:THR:N | 12       | 2.42          |
| (1,33)  | 1:295:A:ILE:C | 1:296:A:SER:N  | 1:296:A:SER:CA | 1:296:A:SER:C | 3        | 2.42          |
| (1,135) | 1:376:A:GLN:C | 1:377:A:ASP:N  | 1:377:A:ASP:CA | 1:377:A:ASP:C | 3        | 2.36          |
| (1,198) | 1:433:A:ARG:N | 1:433:A:ARG:CA | 1:433:A:ARG:C  | 1:434:A:SER:N | 15       | 2.31          |
| (1,131) | 1:373:A:SER:C | 1:374:A:THR:N  | 1:374:A:THR:CA | 1:374:A:THR:C | 1        | 2.26          |
| (1,162) | 1:405:A:ASN:C | 1:406:A:LYS:N  | 1:406:A:LYS:CA | 1:406:A:LYS:C | 13       | 2.18          |
| (1,247) | 1:472:A:TYR:C | 1:473:A:LEU:N  | 1:473:A:LEU:CA | 1:473:A:LEU:C | 9        | 2.13          |
| (1,13)  | 1:278:A:MET:C | 1:279:A:HIS:N  | 1:279:A:HIS:CA | 1:279:A:HIS:C | 12       | 2.08          |
| (1,129) | 1:372:A:ASN:C | 1:373:A:SER:N  | 1:373:A:SER:CA | 1:373:A:SER:C | 11       | 2.04          |
| (1,123) | 1:364:A:GLN:C | 1:365:A:ARG:N  | 1:365:A:ARG:CA | 1:365:A:ARG:C | 11       | 2.03          |
| (1,11)  | 1:277:A:GLY:C | 1:278:A:MET:N  | 1:278:A:MET:CA | 1:278:A:MET:C | 11       | 2.03          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 8        | 2.02          |
| (1,151) | 1:386:A:GLY:N | 1:386:A:GLY:CA | 1:386:A:GLY:C  | 1:387:A:TYR:N | 7        | 2.02          |
| (1,209) | 1:444:A:GLY:C | 1:445:A:GLN:N  | 1:445:A:GLN:CA | 1:445:A:GLN:C | 6        | 2.01          |
| (1,247) | 1:472:A:TYR:C | 1:473:A:LEU:N  | 1:473:A:LEU:CA | 1:473:A:LEU:C | 8        | 1.98          |
| (1,247) | 1:472:A:TYR:C | 1:473:A:LEU:N  | 1:473:A:LEU:CA | 1:473:A:LEU:C | 12       | 1.97          |
| (1,254) | 1:477:A:THR:C | 1:478:A:TRP:N  | 1:478:A:TRP:CA | 1:478:A:TRP:C | 5        | 1.94          |
| (1,196) | 1:432:A:PHE:N | 1:432:A:PHE:CA | 1:432:A:PHE:C  | 1:433:A:ARG:N | 4        | 1.88          |
| (1,198) | 1:433:A:ARG:N | 1:433:A:ARG:CA | 1:433:A:ARG:C  | 1:434:A:SER:N | 4        | 1.87          |
| (1,223) | 1:453:A:MET:C | 1:454:A:LYS:N  | 1:454:A:LYS:CA | 1:454:A:LYS:C | 12       | 1.86          |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 11       | 1.82          |
| (1,276) | 1:491:A:THR:C | 1:492:A:ILE:N  | 1:492:A:ILE:CA | 1:492:A:ILE:C | 13       | 1.81          |
| (1,174) | 1:414:A:GLU:C | 1:415:A:SER:N  | 1:415:A:SER:CA | 1:415:A:SER:C | 9        | 1.76          |
| (1,2)   | 1:259:A:ASN:N | 1:259:A:ASN:CA | 1:259:A:ASN:C  | 1:260:A:ASN:N | 12       | 1.73          |
| (1,224) | 1:454:A:LYS:N | 1:454:A:LYS:CA | 1:454:A:LYS:C  | 1:455:A:GLN:N | 5        | 1.72          |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 8        | 1.71          |
| (1,17)  | 1:280:A:TYR:C | 1:281:A:GLY:N  | 1:281:A:GLY:CA | 1:281:A:GLY:C | 6        | 1.7           |
| (1,2)   | 1:259:A:ASN:N | 1:259:A:ASN:CA | 1:259:A:ASN:C  | 1:260:A:ASN:N | 1        | 1.65          |
| (1,17)  | 1:280:A:TYR:C | 1:281:A:GLY:N  | 1:281:A:GLY:CA | 1:281:A:GLY:C | 8        | 1.62          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,170) | 1:410:A:LEU:C | 1:411:A:TYR:N  | 1:411:A:TYR:CA | 1:411:A:TYR:C | 13       | 1.61          |
| (1,65)  | 1:324:A:ARG:C | 1:325:A:GLN:N  | 1:325:A:GLN:CA | 1:325:A:GLN:C | 11       | 1.6           |
| (1,263) | 1:482:A:THR:N | 1:482:A:THR:CA | 1:482:A:THR:C  | 1:483:A:ASN:N | 11       | 1.58          |
| (1,202) | 1:439:A:GLY:N | 1:439:A:GLY:CA | 1:439:A:GLY:C  | 1:440:A:VAL:N | 8        | 1.56          |
| (1,176) | 1:416:A:ALA:C | 1:417:A:SER:N  | 1:417:A:SER:CA | 1:417:A:SER:C | 1        | 1.56          |
| (1,12)  | 1:278:A:MET:N | 1:278:A:MET:CA | 1:278:A:MET:C  | 1:279:A:HIS:N | 12       | 1.55          |
| (1,247) | 1:472:A:TYR:C | 1:473:A:LEU:N  | 1:473:A:LEU:CA | 1:473:A:LEU:C | 6        | 1.53          |
| (1,8)   | 1:266:A:GLY:N | 1:266:A:GLY:CA | 1:266:A:GLY:C  | 1:267:A:TYR:N | 12       | 1.5           |
| (1,58)  | 1:319:A:ASN:N | 1:319:A:ASN:CA | 1:319:A:ASN:C  | 1:320:A:ASP:N | 14       | 1.49          |
| (1,217) | 1:450:A:ASP:C | 1:451:A:GLU:N  | 1:451:A:GLU:CA | 1:451:A:GLU:C | 5        | 1.48          |
| (1,263) | 1:482:A:THR:N | 1:482:A:THR:CA | 1:482:A:THR:C  | 1:483:A:ASN:N | 15       | 1.46          |
| (1,247) | 1:472:A:TYR:C | 1:473:A:LEU:N  | 1:473:A:LEU:CA | 1:473:A:LEU:C | 13       | 1.46          |
| (1,12)  | 1:278:A:MET:N | 1:278:A:MET:CA | 1:278:A:MET:C  | 1:279:A:HIS:N | 7        | 1.46          |
| (1,113) | 1:356:A:SER:C | 1:357:A:THR:N  | 1:357:A:THR:CA | 1:357:A:THR:C | 3        | 1.45          |
| (1,231) | 1:460:A:TRP:C | 1:461:A:VAL:N  | 1:461:A:VAL:CA | 1:461:A:VAL:C | 1        | 1.43          |
| (1,154) | 1:401:A:GLY:C | 1:402:A:TRP:N  | 1:402:A:TRP:CA | 1:402:A:TRP:C | 1        | 1.43          |
| (1,277) | 1:492:A:ILE:N | 1:492:A:ILE:CA | 1:492:A:ILE:C  | 1:493:A:LYS:N | 3        | 1.37          |
| (1,234) | 1:462:A:GLY:N | 1:462:A:GLY:CA | 1:462:A:GLY:C  | 1:463:A:TYR:N | 5        | 1.34          |
| (1,62)  | 1:321:A:GLY:N | 1:321:A:GLY:CA | 1:321:A:GLY:C  | 1:322:A:VAL:N | 11       | 1.34          |
| (1,247) | 1:472:A:TYR:C | 1:473:A:LEU:N  | 1:473:A:LEU:CA | 1:473:A:LEU:C | 14       | 1.33          |
| (1,31)  | 1:294:A:ALA:C | 1:295:A:ILE:N  | 1:295:A:ILE:CA | 1:295:A:ILE:C | 10       | 1.33          |
| (1,261) | 1:481:A:SER:N | 1:481:A:SER:CA | 1:481:A:SER:C  | 1:482:A:THR:N | 5        | 1.32          |
| (1,37)  | 1:298:A:GLY:C | 1:299:A:LYS:N  | 1:299:A:LYS:CA | 1:299:A:LYS:C | 5        | 1.29          |
| (1,111) | 1:352:A:SER:C | 1:353:A:THR:N  | 1:353:A:THR:CA | 1:353:A:THR:C | 12       | 1.28          |
| (1,187) | 1:423:A:ASP:C | 1:424:A:ILE:N  | 1:424:A:ILE:CA | 1:424:A:ILE:C | 1        | 1.22          |
| (1,209) | 1:444:A:GLY:C | 1:445:A:GLN:N  | 1:445:A:GLN:CA | 1:445:A:GLN:C | 11       | 1.21          |
| (1,277) | 1:492:A:ILE:N | 1:492:A:ILE:CA | 1:492:A:ILE:C  | 1:493:A:LYS:N | 11       | 1.12          |
| (1,111) | 1:352:A:SER:C | 1:353:A:THR:N  | 1:353:A:THR:CA | 1:353:A:THR:C | 14       | 1.12          |
| (1,77)  | 1:332:A:LYS:C | 1:333:A:TYR:N  | 1:333:A:TYR:CA | 1:333:A:TYR:C | 14       | 1.12          |
| (1,273) | 1:490:A:GLY:N | 1:490:A:GLY:CA | 1:490:A:GLY:C  | 1:491:A:THR:N | 15       | 1.09          |
| (1,276) | 1:491:A:THR:C | 1:492:A:ILE:N  | 1:492:A:ILE:CA | 1:492:A:ILE:C | 4        | 1.03          |
| (1,155) | 1:402:A:TRP:N | 1:402:A:TRP:CA | 1:402:A:TRP:C  | 1:403:A:LYS:N | 8        | 1.0           |