



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 01:43 PM UTC

PDB ID : 2LKI / pdb\_00002lki  
BMRB ID : 17995  
Title : Solution NMR structure of holo acyl carrier protein NE2163 from nitrosomonas europaea. Northeast structural genomics consortium target NET1.  
Authors : Lemak, A.; Srisailam, S.; Lukin, J.; Yee, A.; Montecchio, M.; Semesi, A.; Arrowsmith, C.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2011-10-11

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| 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                                                             |

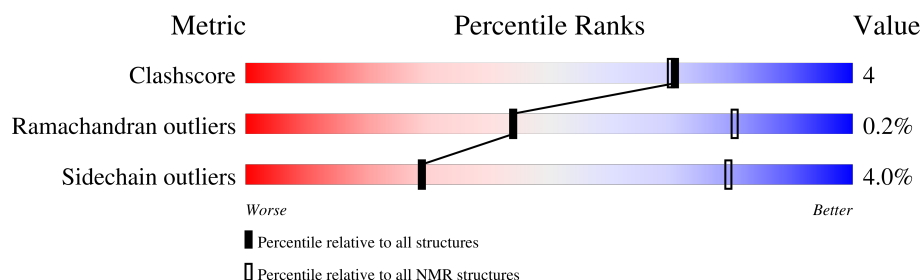
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 90%.

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     | 105    |                  |

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 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: *lowest energy*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:1-A:82 (82)         | 0.49              | 10           |

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 4 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1323 atoms, of which 657 are hydrogens and 0 are deuteriums.

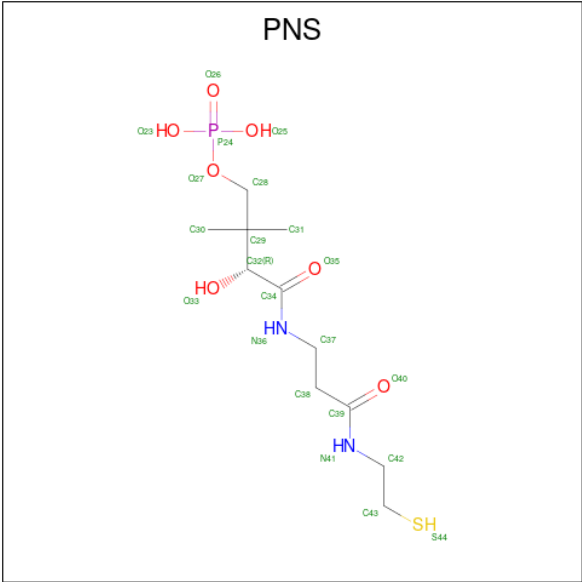
- Molecule 1 is a protein called Putative uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 83       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1281  | 407 | 636 | 105 | 131 | 2 |       |

There are 22 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -21     | MET      | -      | expression tag | UNP Q82SY3 |
| A     | -20     | GLY      | -      | expression tag | UNP Q82SY3 |
| A     | -19     | SER      | -      | expression tag | UNP Q82SY3 |
| A     | -18     | SER      | -      | expression tag | UNP Q82SY3 |
| A     | -17     | HIS      | -      | expression tag | UNP Q82SY3 |
| A     | -16     | HIS      | -      | expression tag | UNP Q82SY3 |
| A     | -15     | HIS      | -      | expression tag | UNP Q82SY3 |
| A     | -14     | HIS      | -      | expression tag | UNP Q82SY3 |
| A     | -13     | HIS      | -      | expression tag | UNP Q82SY3 |
| A     | -12     | HIS      | -      | expression tag | UNP Q82SY3 |
| A     | -11     | SER      | -      | expression tag | UNP Q82SY3 |
| A     | -10     | SER      | -      | expression tag | UNP Q82SY3 |
| A     | -9      | GLY      | -      | expression tag | UNP Q82SY3 |
| A     | -8      | ARG      | -      | expression tag | UNP Q82SY3 |
| A     | -7      | GLU      | -      | expression tag | UNP Q82SY3 |
| A     | -6      | ASN      | -      | expression tag | UNP Q82SY3 |
| A     | -5      | LEU      | -      | expression tag | UNP Q82SY3 |
| A     | -4      | TYR      | -      | expression tag | UNP Q82SY3 |
| A     | -3      | PHE      | -      | expression tag | UNP Q82SY3 |
| A     | -2      | GLN      | -      | expression tag | UNP Q82SY3 |
| A     | -1      | GLY      | -      | expression tag | UNP Q82SY3 |
| A     | 0       | HIS      | -      | expression tag | UNP Q82SY3 |

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>PS).



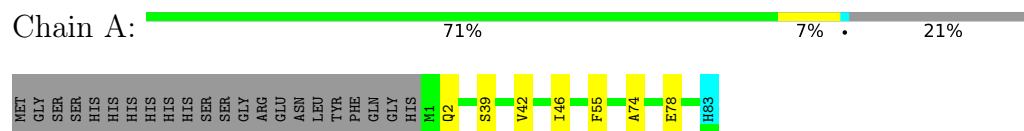
| Mol | Chain | Residues | Atoms |    |    |   |   |   |   |
|-----|-------|----------|-------|----|----|---|---|---|---|
|     |       |          | Total | C  | H  | N | O | P | S |
| 2   | A     | 1        | 42    | 11 | 21 | 2 | 6 | 1 | 1 |

## 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: Putative uncharacterized protein

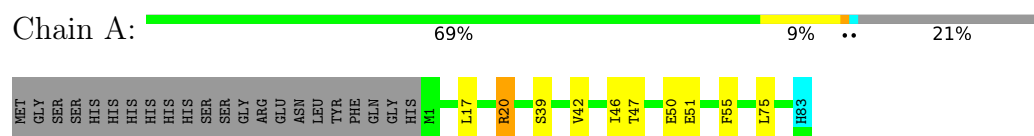


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

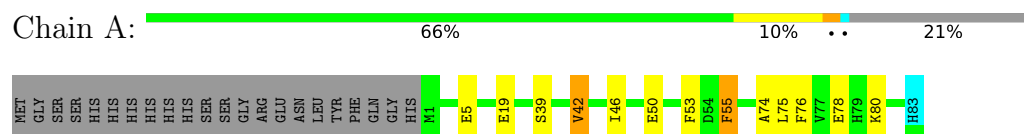
#### 4.2.1 Score per residue for model 1

- Molecule 1: Putative uncharacterized protein



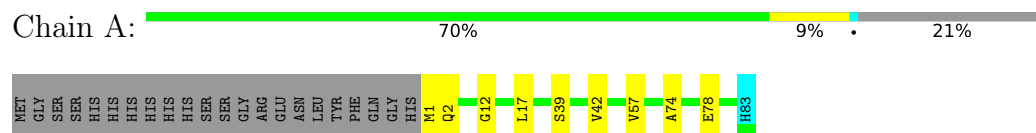
#### 4.2.2 Score per residue for model 2

- Molecule 1: Putative uncharacterized protein



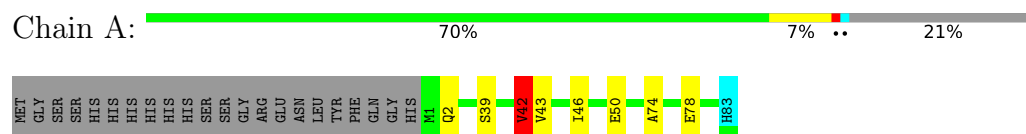
### 4.2.3 Score per residue for model 3

- Molecule 1: Putative uncharacterized protein



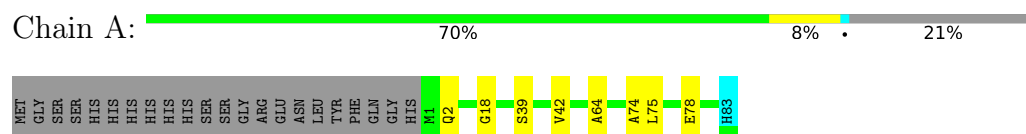
### 4.2.4 Score per residue for model 4

- Molecule 1: Putative uncharacterized protein



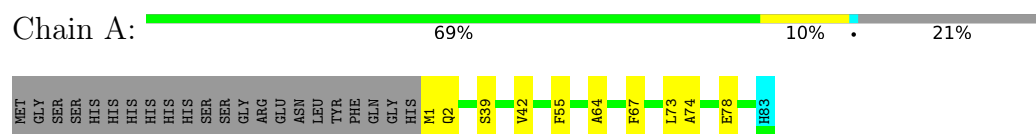
### 4.2.5 Score per residue for model 5

- Molecule 1: Putative uncharacterized protein



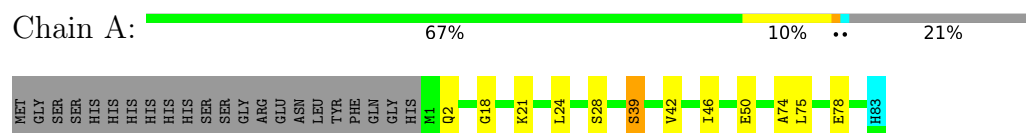
### 4.2.6 Score per residue for model 6

- Molecule 1: Putative uncharacterized protein



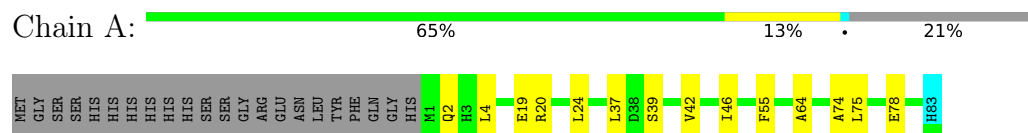
### 4.2.7 Score per residue for model 7

- Molecule 1: Putative uncharacterized protein



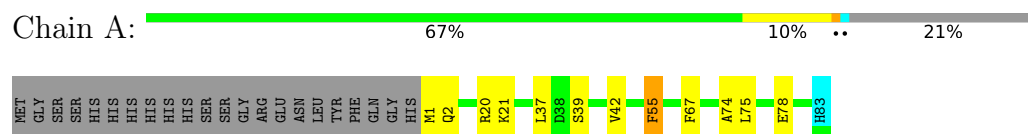
### 4.2.8 Score per residue for model 8

- Molecule 1: Putative uncharacterized protein



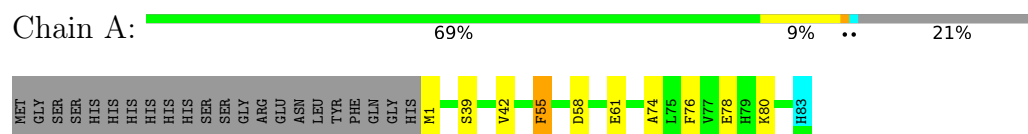
### 4.2.9 Score per residue for model 9

- Molecule 1: Putative uncharacterized protein



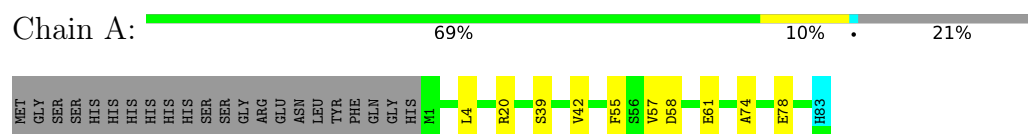
### 4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Putative uncharacterized protein



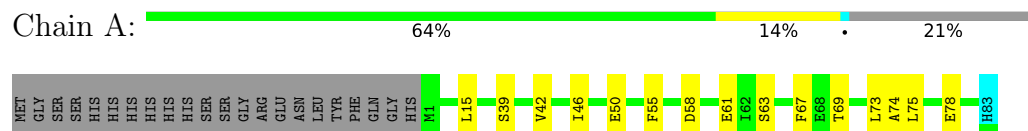
### 4.2.11 Score per residue for model 11

- Molecule 1: Putative uncharacterized protein



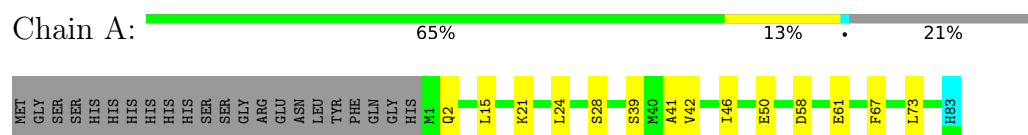
### 4.2.12 Score per residue for model 12

- Molecule 1: Putative uncharacterized protein



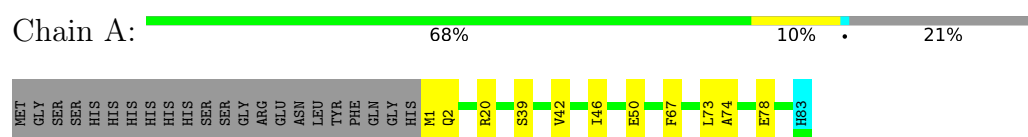
### 4.2.13 Score per residue for model 13

- Molecule 1: Putative uncharacterized protein



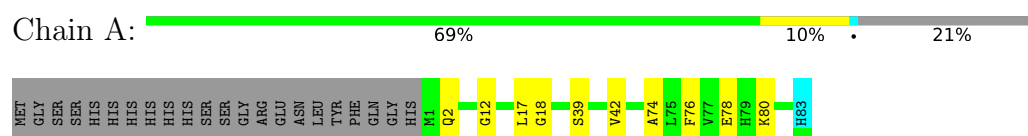
### 4.2.14 Score per residue for model 14

- Molecule 1: Putative uncharacterized protein



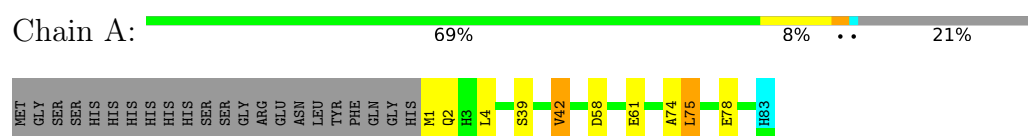
### 4.2.15 Score per residue for model 15

- Molecule 1: Putative uncharacterized protein



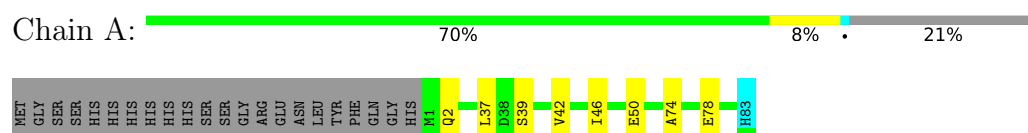
### 4.2.16 Score per residue for model 16

- Molecule 1: Putative uncharacterized protein



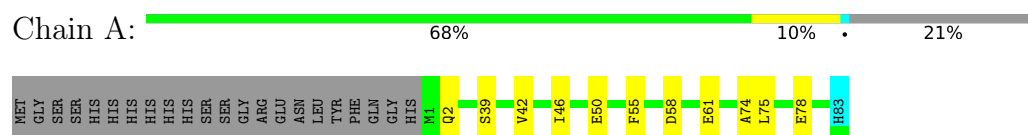
### 4.2.17 Score per residue for model 17

- Molecule 1: Putative uncharacterized protein



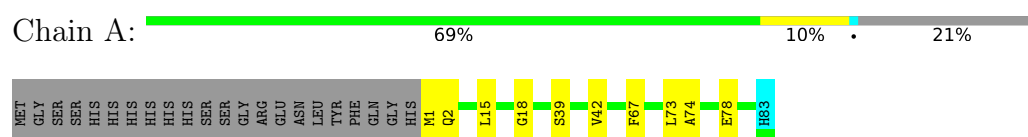
#### 4.2.18 Score per residue for model 18

- Molecule 1: Putative uncharacterized protein



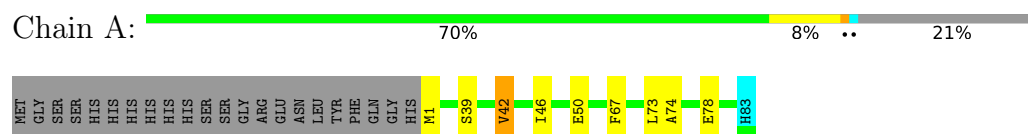
#### 4.2.19 Score per residue for model 19

- Molecule 1: Putative uncharacterized protein



#### 4.2.20 Score per residue for model 20

- Molecule 1: Putative uncharacterized protein



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution |         |
| CNS           | 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               | 2              |
| Total number of shifts                       | 1033           |
| Number of shifts mapped to atoms             | 1033           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 90%            |

## 6 Model quality [i](#)

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

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

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 1.25±0.02    | 0±0/643 ( 0.0± 0.1%) | 1.04±0.02   | 0±0/874 ( 0.0± 0.0%) |
| All | All   | 1.25         | 3/12860 ( 0.0%)      | 1.04        | 2/17480 ( 0.0%)      |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 1   | A     | 42  | VAL  | CA-CB | 5.03 | 1.60        | 1.54     | 4      | 3     |

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|----------|------|-------------|----------|--------|-------|
|     |       |     |      |          |      |             |          | Worst  | Total |
| 1   | A     | 55  | PHE  | CA-CB-CG | 5.62 | 119.42      | 113.80   | 10     | 2     |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 634   | 628      | 627      | 4±1     |
| 2   | A     | 21    | 21       | 21       | 1±1     |
| All | All   | 13100 | 12980    | 12960    | 92      |

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 4.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:39:SER:O    | 1:A:42:VAL:HG22 | 0.60     | 1.97        | 10     | 20    |
| 1:A:39:SER:HB3  | 2:A:84:PNS:H282 | 0.53     | 1.80        | 5      | 5     |
| 1:A:1:MET:SD    | 1:A:78:GLU:HG3  | 0.52     | 2.45        | 19     | 1     |
| 1:A:67:PHE:HB2  | 2:A:84:PNS:S44  | 0.50     | 2.46        | 9      | 1     |
| 1:A:74:ALA:O    | 1:A:78:GLU:HG2  | 0.50     | 2.07        | 11     | 18    |
| 1:A:67:PHE:HA   | 1:A:73:LEU:HD21 | 0.49     | 1.84        | 19     | 6     |
| 1:A:39:SER:HB2  | 2:A:84:PNS:H301 | 0.48     | 1.84        | 10     | 1     |
| 1:A:58:ASP:O    | 1:A:61:GLU:HG2  | 0.48     | 2.08        | 12     | 6     |
| 1:A:64:ALA:HA   | 2:A:84:PNS:S44  | 0.47     | 2.49        | 5      | 3     |
| 1:A:24:LEU:HB2  | 1:A:28:SER:HB2  | 0.47     | 1.87        | 13     | 2     |
| 2:A:84:PNS:O26  | 2:A:84:PNS:H302 | 0.46     | 2.10        | 5      | 1     |
| 1:A:46:ILE:O    | 1:A:50:GLU:HG2  | 0.46     | 2.11        | 4      | 10    |
| 1:A:15:LEU:HD11 | 1:A:41:ALA:HB1  | 0.45     | 1.87        | 13     | 1     |
| 1:A:1:MET:HE2   | 1:A:75:LEU:HD21 | 0.44     | 1.88        | 9      | 1     |
| 2:A:84:PNS:H36  | 2:A:84:PNS:H313 | 0.43     | 1.74        | 4      | 1     |
| 1:A:17:LEU:HB3  | 1:A:20:ARG:HB3  | 0.43     | 1.91        | 1      | 1     |
| 1:A:67:PHE:CD1  | 2:A:84:PNS:S44  | 0.42     | 3.11        | 12     | 1     |
| 1:A:63:SER:O    | 2:A:84:PNS:S44  | 0.42     | 2.78        | 12     | 1     |
| 1:A:43:VAL:HG21 | 2:A:84:PNS:H312 | 0.41     | 1.91        | 4      | 1     |
| 1:A:76:PHE:O    | 1:A:80:LYS:HG2  | 0.41     | 2.15        | 2      | 3     |
| 1:A:12:GLY:HA2  | 1:A:17:LEU:HB2  | 0.41     | 1.92        | 3      | 2     |
| 1:A:42:VAL:O    | 1:A:46:ILE:HG13 | 0.41     | 2.15        | 8      | 1     |
| 1:A:53:PHE:HB2  | 1:A:55:PHE:CD1  | 0.41     | 2.51        | 2      | 1     |
| 1:A:1:MET:HE2   | 1:A:75:LEU:HD22 | 0.41     | 1.93        | 16     | 1     |
| 1:A:20:ARG:NH1  | 1:A:24:LEU:HB3  | 0.40     | 2.31        | 8      | 1     |
| 1:A:47:THR:O    | 1:A:51:GLU:HG2  | 0.40     | 2.16        | 1      | 1     |
| 1:A:55:PHE:CZ   | 1:A:57:VAL:HG22 | 0.40     | 2.51        | 11     | 1     |

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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

| Mol | Chain | Analysed        | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|------------|-------------|----|
| 1   | A     | 81/105 (77%)    | 75±1 (93±2%) | 5±1 (7±2%) | 0±0 (0±0%) | 44          | 80 |
| All | All   | 1620/2100 (77%) | 1508 (93%)   | 108 (7%)   | 4 (0%)     | 44          | 80 |

All 1 unique Ramachandran outliers are listed below.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 18  | GLY  | 4              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|-------------|----|
| 1   | A     | 72/92 (78%)     | 69±1 (96±2%) | 3±1 (4±2%) | 29          | 79 |
| All | All   | 1440/1840 (78%) | 1382 (96%)   | 58 (4%)    | 29          | 79 |

All 15 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     | 2   | GLN  | 14             |
| 1   | A     | 55  | PHE  | 8              |
| 1   | A     | 75  | LEU  | 8              |
| 1   | A     | 1   | MET  | 5              |
| 1   | A     | 20  | ARG  | 4              |
| 1   | A     | 21  | LYS  | 3              |
| 1   | A     | 4   | LEU  | 3              |
| 1   | A     | 37  | LEU  | 3              |
| 1   | A     | 19  | GLU  | 2              |
| 1   | A     | 42  | VAL  | 2              |
| 1   | A     | 15  | LEU  | 2              |
| 1   | A     | 5   | GLU  | 1              |
| 1   | A     | 57  | VAL  | 1              |
| 1   | A     | 39  | SER  | 1              |
| 1   | A     | 69  | THR  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |           |            |
|-----|------|-------|-----|------|--------------|-----------|------------|
|     |      |       |     |      | Counts       | RMSZ      | #Z>2       |
| 2   | PNS  | A     | 84  | 1    | 14,20,21     | 1.18±0.09 | 1±0 (7±0%) |

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

| Mol | Type | Chain | Res | Link | Bond angles |           |            |
|-----|------|-------|-----|------|-------------|-----------|------------|
|     |      |       |     |      | Counts      | RMSZ      | #Z>2       |
| 2   | PNS  | A     | 84  | 1    | 18,26,29    | 0.80±0.13 | 1±0 (3±2%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings |
|-----|------|-------|-----|------|---------|--------------|-------|
| 2   | PNS  | A     | 84  | 1    | -       | 0±0,24,26,27 | -     |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
|     |       |     |      |         |      |             |          | Worst  | Total |
| 2   | A     | 84  | PNS  | C28-C29 | 4.41 | 1.59        | 1.52     | 1      | 20    |

All unique angle outliers are listed below.

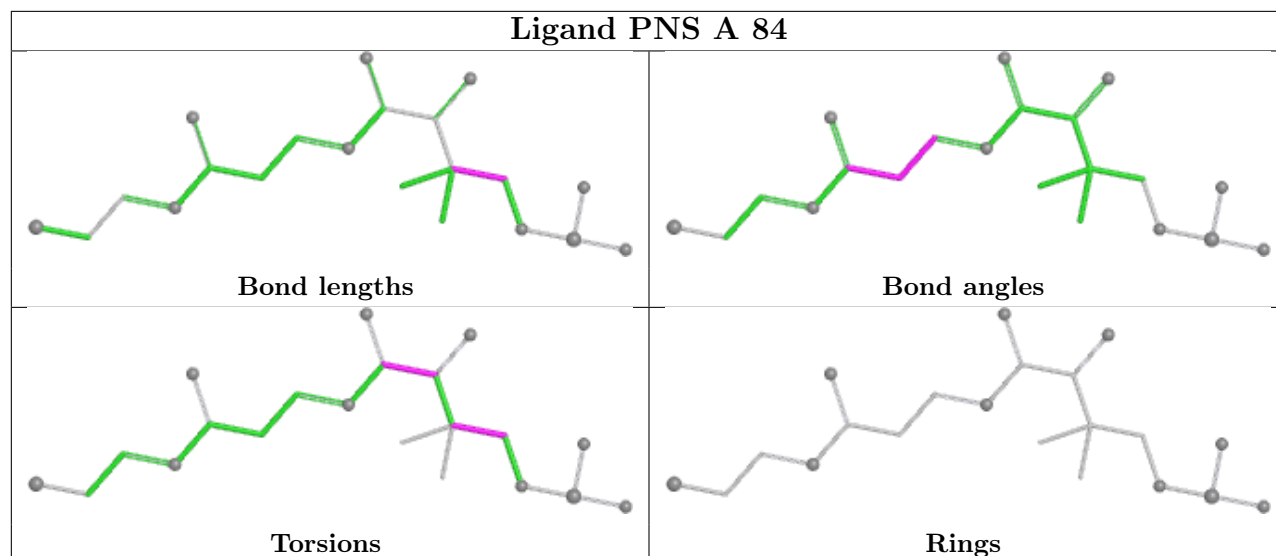
| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
|     |       |     |      |             |      |             |          | Worst  | Total |
| 2   | A     | 84  | PNS  | C37-C38-C39 | 3.13 | 117.61      | 112.39   | 12     | 12    |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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 90% for the well-defined parts and 90% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1004 |
| Number of shifts mapped to atoms        | 1004 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 1    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 83       | $-0.47 \pm 0.32$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 78       | $0.10 \pm 0.16$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 78       | $-0.17 \pm 0.23$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 78       | $-0.23 \pm 0.34$                | 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 90%, i.e. 997 atoms were assigned a chemical shift out of a possible 1104. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 400/412 (97%) | 163/167 (98%) | 160/164 (98%)   | 77/81 (95%)     |
| Sidechain | 558/619 (90%) | 383/407 (94%) | 169/198 (85%)   | 6/14 (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 | 39/73 (53%)    | 24/36 (67%)          | 15/31 (48%)           | 0/6 (0%)              |
| Overall  | 997/1104 (90%) | 570/610 (93%)        | 344/393 (88%)         | 83/101 (82%)          |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1004 atoms were assigned a chemical shift out of a possible 1120. 0 out of 21 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  | 404/417 (97%)   | 165/169 (98%)        | 161/166 (97%)         | 78/82 (95%)           |
| Sidechain | 561/622 (90%)   | 385/409 (94%)        | 170/199 (85%)         | 6/14 (43%)            |
| Aromatic  | 39/81 (48%)     | 24/40 (60%)          | 15/33 (45%)           | 0/8 (0%)              |
| Overall   | 1004/1120 (90%) | 574/618 (93%)        | 346/398 (87%)         | 84/104 (81%)          |

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

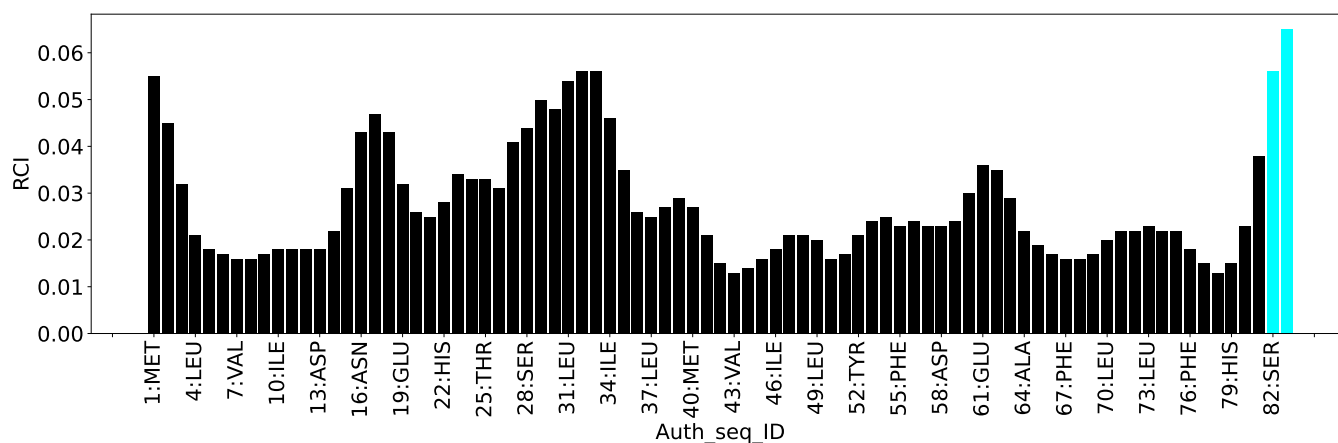
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 80  | LYS  | HG3  | 0.03       | 0.04 – 2.67         | -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:



## 7.2 Chemical shift list 2

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

### 7.2.1 Bookkeeping [i](#)

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                  | 29 |
| Number of shifts mapped to atoms        | 29 |
| Number of unparsed shifts               | 0  |
| Number of shifts with mapping errors    | 0  |
| Number of shifts with mapping warnings  | 0  |
| Number of shift outliers (ShiftChecker) | 0  |

### 7.2.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

### 7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1104. 0 out of 21 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 | 0/412 (0%)   | 0/167 (0%)           | 0/164 (0%)            | 0/81 (0%)             |

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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> |
|-----------|--------------|----------------------|-----------------------|-----------------------|
| Sidechain | 0/619 (0%)   | 0/407 (0%)           | 0/198 (0%)            | 0/14 (0%)             |
| Aromatic  | 0/73 (0%)    | 0/36 (0%)            | 0/31 (0%)             | 0/6 (0%)              |
| Overall   | 0/1104 (0%)  | 0/610 (0%)           | 0/393 (0%)            | 0/101 (0%)            |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1120. 0 out of 21 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  | 0/417 (0%)   | 0/169 (0%)           | 0/166 (0%)            | 0/82 (0%)             |
| Sidechain | 0/622 (0%)   | 0/409 (0%)           | 0/199 (0%)            | 0/14 (0%)             |
| Aromatic  | 0/81 (0%)    | 0/40 (0%)            | 0/33 (0%)             | 0/8 (0%)              |
| Overall   | 0/1120 (0%)  | 0/618 (0%)           | 0/398 (0%)            | 0/104 (0%)            |

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

There are no statistically unusual chemical shifts.

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

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins

## 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                                | 2104  |
| Intra-residue ( $ i-j =0$ )                              | 445   |
| Sequential ( $ i-j =1$ )                                 | 531   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 535   |
| Long range ( $ i-j \geq 5$ )                             | 449   |
| Inter-chain                                              | 50    |
| Hydrogen bond restraints                                 | 94    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 146   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 21.2  |
| Number of long range restraints per residue <sup>1</sup> | 4.2   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 25.6                                   | 0.2     |
| 0.2-0.5 (Medium) | 6.3                                    | 0.47    |
| >0.5 (Large)     | 0.1                                    | 0.56    |

### 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)   | 4.2                                    | 6.19    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis

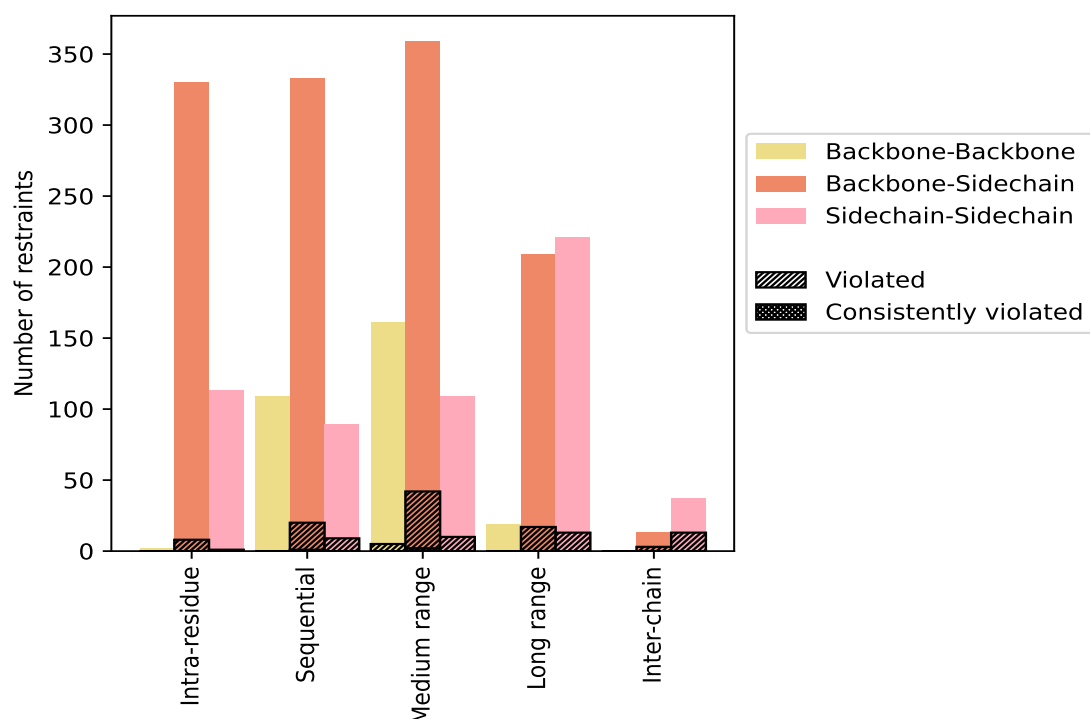
### 9.1 Summary of distance violations

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

| Restrains type                         | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|----------------------------------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                        |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| Intra-residue ( $ i-j =0$ )            | 445   | 21.2           | 9                     | 2.0            | 0.4            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 2     | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 330   | 15.7           | 8                     | 2.4            | 0.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 113   | 5.4            | 1                     | 0.9            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sequential ( $ i-j =1$ )               | 531   | 25.2           | 29                    | 5.5            | 1.4            | 1                                  | 0.2            | 0.0            |
| Backbone-Backbone                      | 109   | 5.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 333   | 15.8           | 20                    | 6.0            | 1.0            | 1                                  | 0.3            | 0.0            |
| Sidechain-Sidechain                    | 89    | 4.2            | 9                     | 10.1           | 0.4            | 0                                  | 0.0            | 0.0            |
| Medium range ( $ i-j >1$ & $ i-j <5$ ) | 535   | 25.4           | 30                    | 5.6            | 1.4            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 161   | 7.7            | 5                     | 3.1            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 265   | 12.6           | 15                    | 5.7            | 0.7            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 109   | 5.2            | 10                    | 9.2            | 0.5            | 0                                  | 0.0            | 0.0            |
| Long range ( $ i-j \geq 5$ )           | 449   | 21.3           | 30                    | 6.7            | 1.4            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 19    | 0.9            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 209   | 9.9            | 17                    | 8.1            | 0.8            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 221   | 10.5           | 13                    | 5.9            | 0.6            | 0                                  | 0.0            | 0.0            |
| Inter-chain                            | 50    | 2.4            | 16                    | 32.0           | 0.8            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 13    | 0.6            | 3                     | 23.1           | 0.1            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 37    | 1.8            | 13                    | 35.1           | 0.6            | 0                                  | 0.0            | 0.0            |
| Hydrogen bond                          | 94    | 4.5            | 27                    | 28.7           | 1.3            | 2                                  | 2.1            | 0.1            |
| Disulfide bond                         | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total                                  | 2104  | 100.0          | 141                   | 6.7            | 6.7            | 3                                  | 0.1            | 0.1            |
| Backbone-Backbone                      | 291   | 13.8           | 5                     | 1.7            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 1244  | 59.1           | 90                    | 7.2            | 4.3            | 3                                  | 0.2            | 0.1            |
| Sidechain-Sidechain                    | 569   | 27.0           | 46                    | 8.1            | 2.2            | 0                                  | 0.0            | 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 disulfide 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                    | 7               | 16              | 3               | 4               | 31    | 0.17     | 0.39    | 0.07                | 0.15       |
| 2        | 2                    | 6               | 19              | 8               | 3               | 38    | 0.16     | 0.36    | 0.06                | 0.15       |
| 3        | 2                    | 9               | 13              | 6               | 5               | 35    | 0.16     | 0.43    | 0.06                | 0.15       |
| 4        | 3                    | 4               | 14              | 4               | 3               | 28    | 0.18     | 0.44    | 0.08                | 0.15       |
| 5        | 1                    | 10              | 11              | 7               | 6               | 35    | 0.17     | 0.43    | 0.07                | 0.16       |
| 6        | 1                    | 6               | 16              | 8               | 1               | 32    | 0.15     | 0.42    | 0.06                | 0.13       |
| 7        | 3                    | 10              | 20              | 6               | 4               | 43    | 0.16     | 0.31    | 0.05                | 0.14       |
| 8        | 1                    | 7               | 27              | 2               | 3               | 40    | 0.16     | 0.45    | 0.07                | 0.13       |
| 9        | 0                    | 7               | 20              | 4               | 6               | 37    | 0.17     | 0.43    | 0.08                | 0.13       |
| 10       | 1                    | 8               | 17              | 5               | 5               | 36    | 0.18     | 0.44    | 0.07                | 0.16       |

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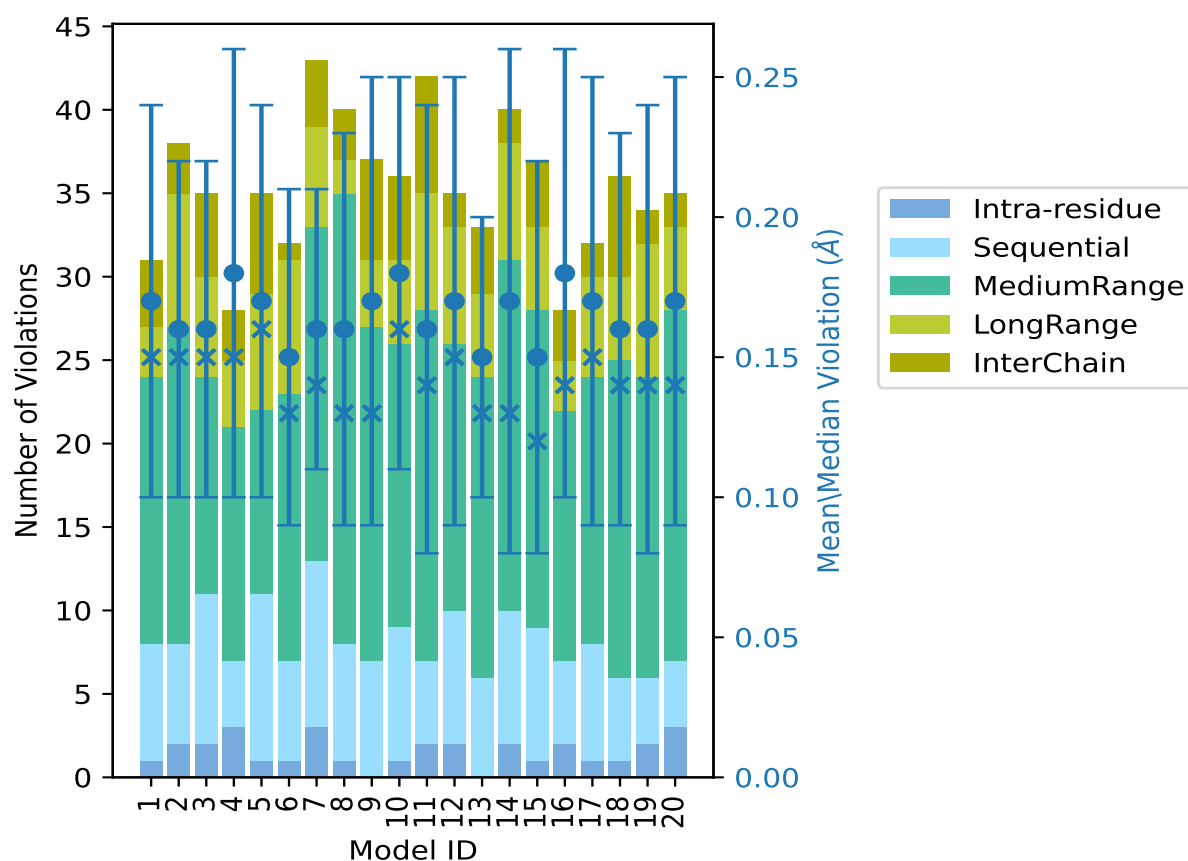
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 2                    | 5               | 21              | 7               | 7               | 42    | 0.16     | 0.56    | 0.08                | 0.14       |
| 12       | 2                    | 8               | 16              | 7               | 2               | 35    | 0.17     | 0.45    | 0.08                | 0.15       |
| 13       | 0                    | 6               | 18              | 5               | 4               | 33    | 0.15     | 0.32    | 0.05                | 0.13       |
| 14       | 2                    | 8               | 21              | 7               | 2               | 40    | 0.17     | 0.47    | 0.09                | 0.13       |
| 15       | 1                    | 8               | 19              | 5               | 4               | 37    | 0.15     | 0.4     | 0.07                | 0.12       |
| 16       | 2                    | 5               | 15              | 3               | 3               | 28    | 0.18     | 0.41    | 0.08                | 0.14       |
| 17       | 1                    | 7               | 16              | 6               | 2               | 32    | 0.17     | 0.43    | 0.08                | 0.15       |
| 18       | 1                    | 5               | 19              | 5               | 6               | 36    | 0.16     | 0.45    | 0.07                | 0.14       |
| 19       | 2                    | 4               | 18              | 8               | 2               | 34    | 0.16     | 0.43    | 0.08                | 0.14       |
| 20       | 3                    | 4               | 21              | 5               | 2               | 35    | 0.17     | 0.44    | 0.08                | 0.14       |

<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

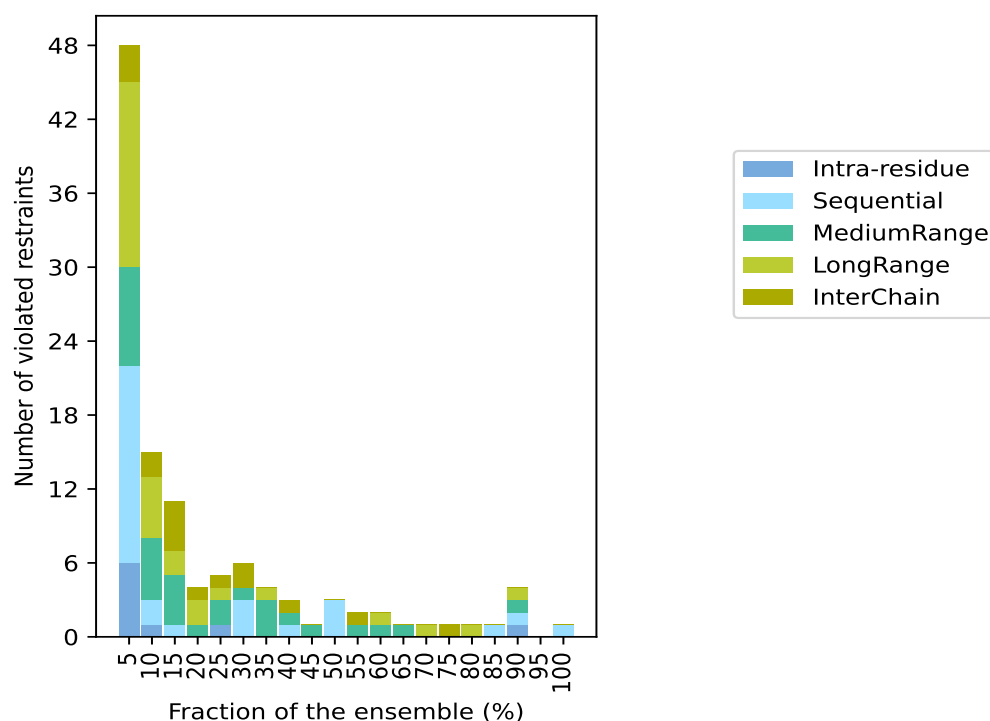
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1896(IR:436, SQ:502, MR:505, LR:419, IC:34) restraints are 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>       | %     |
| 6                             | 16              | 8               | 15              | 3               | 48    | 1                        | 5.0   |
| 1                             | 2               | 5               | 5               | 2               | 15    | 2                        | 10.0  |
| 0                             | 1               | 4               | 2               | 4               | 11    | 3                        | 15.0  |
| 0                             | 0               | 1               | 2               | 1               | 4     | 4                        | 20.0  |
| 1                             | 0               | 2               | 1               | 1               | 5     | 5                        | 25.0  |
| 0                             | 3               | 1               | 0               | 2               | 6     | 6                        | 30.0  |
| 0                             | 0               | 3               | 1               | 0               | 4     | 7                        | 35.0  |
| 0                             | 1               | 1               | 0               | 1               | 3     | 8                        | 40.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 9                        | 45.0  |
| 0                             | 3               | 0               | 0               | 0               | 3     | 10                       | 50.0  |
| 0                             | 0               | 1               | 0               | 1               | 2     | 11                       | 55.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 12                       | 60.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 13                       | 65.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 14                       | 70.0  |
| 0                             | 0               | 0               | 0               | 1               | 1     | 15                       | 75.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 16                       | 80.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 17                       | 85.0  |
| 1                             | 1               | 1               | 1               | 0               | 4     | 18                       | 90.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 19                       | 95.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 20                       | 100.0 |

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

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

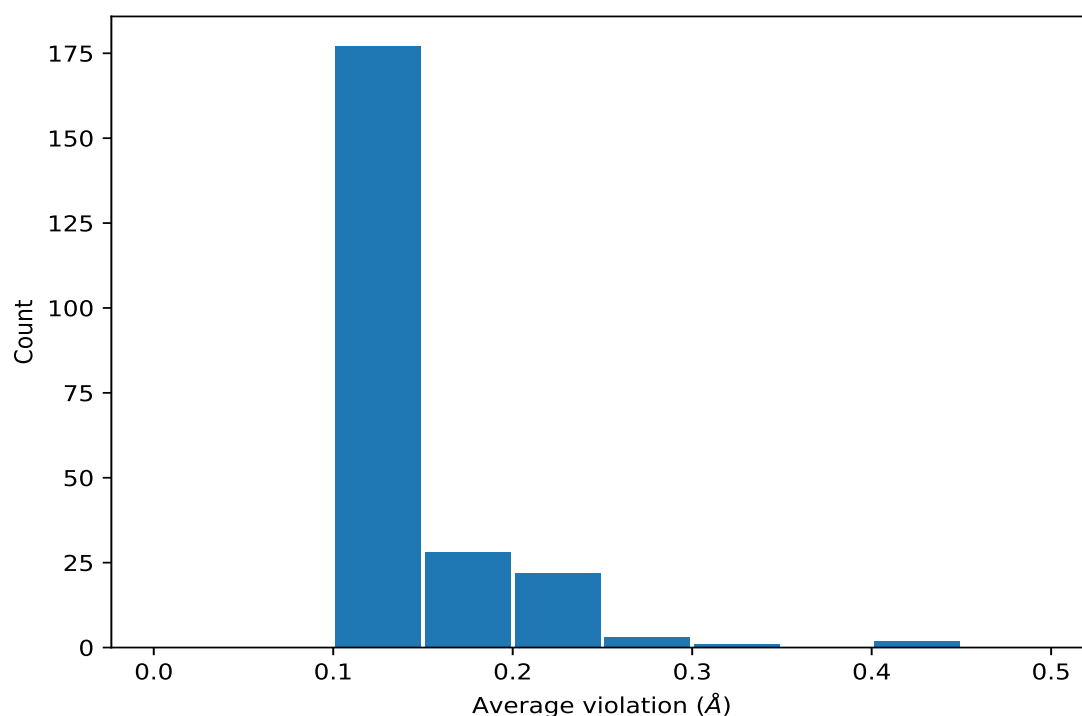
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 20                  | 0.34     | 0.06                | 0.36       |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 20                  | 0.21     | 0.05                | 0.22       |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 20                  | 0.16     | 0.02                | 0.15       |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 20                  | 0.16     | 0.02                | 0.15       |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 20                  | 0.16     | 0.02                | 0.15       |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 19                  | 0.16     | 0.02                | 0.15       |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 18                  | 0.42     | 0.06                | 0.43       |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 18                  | 0.42     | 0.06                | 0.43       |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 18                  | 0.22     | 0.05                | 0.22       |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 18                  | 0.22     | 0.05                | 0.22       |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 18                  | 0.22     | 0.05                | 0.22       |
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 18                  | 0.17     | 0.04                | 0.16       |
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 18                  | 0.17     | 0.04                | 0.16       |
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 18                  | 0.17     | 0.04                | 0.16       |
| (1,456)  | 1:34:A:ILE:HB   | 1:36:A:GLU:H    | 18                  | 0.16     | 0.02                | 0.16       |
| (2,61)   | 1:73:A:LEU:H    | 1:69:A:THR:O    | 18                  | 0.13     | 0.02                | 0.13       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 17                  | 0.14     | 0.03                | 0.14       |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 17                  | 0.14     | 0.03                | 0.14       |
| (1,933)  | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3  | 17                  | 0.14     | 0.03                | 0.14       |
| (1,833)  | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 16                  | 0.16     | 0.04                | 0.15       |
| (2,81)   | 1:13:A:ASP:H    | 1:9:A:ASN:O     | 16                  | 0.14     | 0.03                | 0.14       |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 15                  | 0.24     | 0.06                | 0.24       |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 15                  | 0.24     | 0.06                | 0.24       |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 15                  | 0.24     | 0.06                | 0.24       |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 15                  | 0.24     | 0.06                | 0.24       |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 15                  | 0.24     | 0.06                | 0.24       |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 15                  | 0.24     | 0.06                | 0.24       |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 15                  | 0.24     | 0.06                | 0.24       |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 15                  | 0.24     | 0.06                | 0.24       |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 15                  | 0.24     | 0.06                | 0.24       |
| (2,73)   | 1:79:A:HIS:H    | 1:75:A:LEU:O    | 15                  | 0.14     | 0.04                | 0.13       |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 14                  | 0.14     | 0.03                | 0.15       |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 14                  | 0.14     | 0.03                | 0.15       |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 14                  | 0.14     | 0.03                | 0.15       |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 14                  | 0.14     | 0.03                | 0.15       |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 14                  | 0.14     | 0.03                | 0.15       |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 14                  | 0.14     | 0.03                | 0.15       |
| (2,1)    | 1:3:A:HIS:O     | 1:7:A:VAL:H     | 14                  | 0.12     | 0.01                | 0.12       |
| (1,185)  | 1:4:A:LEU:H     | 1:7:A:VAL:HB    | 13                  | 0.14     | 0.02                | 0.14       |
| (2,2)    | 1:3:A:HIS:O     | 1:7:A:VAL:N     | 13                  | 0.12     | 0.03                | 0.11       |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB1  | 12                  | 0.19     | 0.03                | 0.19       |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB2  | 12                  | 0.19     | 0.03                | 0.19       |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB3  | 12                  | 0.19     | 0.03                | 0.19       |
| (1,44)   | 1:40:A:MET:HB3  | 1:43:A:VAL:H    | 12                  | 0.15     | 0.03                | 0.15       |
| (2,43)   | 1:46:A:ILE:H    | 1:42:A:VAL:O    | 12                  | 0.13     | 0.02                | 0.12       |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG21 | 11                  | 0.17     | 0.06                | 0.16       |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG22 | 11                  | 0.17     | 0.06                | 0.16       |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG23 | 11                  | 0.17     | 0.06                | 0.16       |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG21 | 11                  | 0.17     | 0.06                | 0.16       |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG22 | 11                  | 0.17     | 0.06                | 0.16       |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG23 | 11                  | 0.17     | 0.06                | 0.16       |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG21  | 11                  | 0.16     | 0.04                | 0.15       |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG22  | 11                  | 0.16     | 0.04                | 0.15       |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG23  | 11                  | 0.16     | 0.04                | 0.15       |
| (1,741)  | 1:8:A:ARG:HG3   | 1:9:A:ASN:HA    | 10                  | 0.17     | 0.05                | 0.17       |
| (1,1021) | 1:45:A:VAL:HB   | 1:46:A:ILE:HG13 | 10                  | 0.15     | 0.04                | 0.16       |
| (1,1722) | 1:4:A:LEU:HD11  | 1:5:A:GLU:HA    | 10                  | 0.14     | 0.02                | 0.14       |
| (1,1722) | 1:4:A:LEU:HD12  | 1:5:A:GLU:HA    | 10                  | 0.14     | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1722) | 1:4:A:LEU:HD13  | 1:5:A:GLU:HA    | 10                  | 0.14     | 0.02                | 0.14       |
| (1,1722) | 1:4:A:LEU:HD21  | 1:5:A:GLU:HA    | 10                  | 0.14     | 0.02                | 0.14       |
| (1,1722) | 1:4:A:LEU:HD22  | 1:5:A:GLU:HA    | 10                  | 0.14     | 0.02                | 0.14       |
| (1,1722) | 1:4:A:LEU:HD23  | 1:5:A:GLU:HA    | 10                  | 0.14     | 0.02                | 0.14       |
| (2,28)   | 1:76:A:PHE:O    | 1:80:A:LYS:N    | 10                  | 0.13     | 0.03                | 0.12       |
| (1,772)  | 1:10:A:ILE:HG21 | 1:13:A:ASP:HB2  | 9                   | 0.13     | 0.03                | 0.12       |
| (1,772)  | 1:10:A:ILE:HG22 | 1:13:A:ASP:HB2  | 9                   | 0.13     | 0.03                | 0.12       |
| (1,772)  | 1:10:A:ILE:HG23 | 1:13:A:ASP:HB2  | 9                   | 0.13     | 0.03                | 0.12       |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG11 | 8                   | 0.21     | 0.07                | 0.2        |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG12 | 8                   | 0.21     | 0.07                | 0.2        |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG13 | 8                   | 0.21     | 0.07                | 0.2        |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG11 | 8                   | 0.21     | 0.07                | 0.2        |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG12 | 8                   | 0.21     | 0.07                | 0.2        |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG13 | 8                   | 0.21     | 0.07                | 0.2        |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG2   | 8                   | 0.18     | 0.04                | 0.17       |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG3   | 8                   | 0.18     | 0.04                | 0.17       |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG2   | 8                   | 0.18     | 0.04                | 0.17       |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG3   | 8                   | 0.18     | 0.04                | 0.17       |
| (1,649)  | 1:6:A:ALA:HB1   | 1:9:A:ASN:HD22  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,649)  | 1:6:A:ALA:HB2   | 1:9:A:ASN:HD22  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,649)  | 1:6:A:ALA:HB3   | 1:9:A:ASN:HD22  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,22)   | 1:55:A:PHE:HD1  | 1:58:A:ASP:H    | 7                   | 0.23     | 0.08                | 0.25       |
| (1,22)   | 1:55:A:PHE:HD2  | 1:58:A:ASP:H    | 7                   | 0.23     | 0.08                | 0.25       |
| (1,7)    | 1:2:A:GLN:HE21  | 1:4:A:LEU:H     | 7                   | 0.18     | 0.04                | 0.16       |
| (1,256)  | 1:1:A:MET:HG3   | 1:4:A:LEU:H     | 7                   | 0.15     | 0.06                | 0.12       |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD11 | 7                   | 0.14     | 0.05                | 0.12       |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD12 | 7                   | 0.14     | 0.05                | 0.12       |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD13 | 7                   | 0.14     | 0.05                | 0.12       |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD21 | 7                   | 0.14     | 0.05                | 0.12       |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD22 | 7                   | 0.14     | 0.05                | 0.12       |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD23 | 7                   | 0.14     | 0.05                | 0.12       |
| (2,93)   | 1:67:A:PHE:H    | 1:64:A:ALA:O    | 7                   | 0.13     | 0.03                | 0.12       |
| (2,75)   | 1:80:A:LYS:H    | 1:76:A:PHE:O    | 7                   | 0.12     | 0.01                | 0.12       |
| (1,1711) | 1:2:A:GLN:HG2   | 1:3:A:HIS:HA    | 6                   | 0.27     | 0.04                | 0.27       |
| (1,1711) | 1:2:A:GLN:HG3   | 1:3:A:HIS:HA    | 6                   | 0.27     | 0.04                | 0.27       |
| (1,1388) | 1:24:A:LEU:HD11 | 1:25:A:THR:HA   | 6                   | 0.14     | 0.02                | 0.14       |
| (1,1388) | 1:24:A:LEU:HD12 | 1:25:A:THR:HA   | 6                   | 0.14     | 0.02                | 0.14       |
| (1,1388) | 1:24:A:LEU:HD13 | 1:25:A:THR:HA   | 6                   | 0.14     | 0.02                | 0.14       |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 6                   | 0.13     | 0.04                | 0.12       |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 6                   | 0.13     | 0.04                | 0.12       |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 6                   | 0.13     | 0.04                | 0.12       |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 6                   | 0.13     | 0.04                | 0.12       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 6                   | 0.13     | 0.04                | 0.12       |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 6                   | 0.13     | 0.04                | 0.12       |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 6                   | 0.13     | 0.04                | 0.12       |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 6                   | 0.13     | 0.04                | 0.12       |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 6                   | 0.13     | 0.04                | 0.12       |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 6                   | 0.13     | 0.04                | 0.12       |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 6                   | 0.13     | 0.04                | 0.12       |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 6                   | 0.13     | 0.04                | 0.12       |
| (1,299)  | 1:13:A:ASP:HA   | 1:15:A:LEU:H    | 6                   | 0.13     | 0.03                | 0.12       |
| (1,106)  | 1:80:A:LYS:HD2  | 1:81:A:LEU:H    | 6                   | 0.12     | 0.01                | 0.12       |
| (2,33)   | 1:9:A:ASN:H     | 1:5:A:GLU:O     | 6                   | 0.12     | 0.01                | 0.12       |
| (1,75)   | 1:16:A:ASN:H    | 1:16:A:ASN:HD21 | 5                   | 0.27     | 0.11                | 0.24       |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG21 | 5                   | 0.14     | 0.03                | 0.14       |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG22 | 5                   | 0.14     | 0.03                | 0.14       |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG23 | 5                   | 0.14     | 0.03                | 0.14       |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG21 | 5                   | 0.14     | 0.03                | 0.14       |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG22 | 5                   | 0.14     | 0.03                | 0.14       |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG23 | 5                   | 0.14     | 0.03                | 0.14       |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD11 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD12 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD13 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD11 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD12 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD13 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD11 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD12 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD13 | 5                   | 0.14     | 0.02                | 0.14       |
| (1,1600) | 1:49:A:LEU:HD11 | 1:52:A:TYR:HD1  | 5                   | 0.13     | 0.02                | 0.14       |
| (1,1600) | 1:49:A:LEU:HD11 | 1:52:A:TYR:HD2  | 5                   | 0.13     | 0.02                | 0.14       |
| (1,1600) | 1:49:A:LEU:HD12 | 1:52:A:TYR:HD1  | 5                   | 0.13     | 0.02                | 0.14       |
| (1,1600) | 1:49:A:LEU:HD12 | 1:52:A:TYR:HD2  | 5                   | 0.13     | 0.02                | 0.14       |
| (1,1600) | 1:49:A:LEU:HD13 | 1:52:A:TYR:HD1  | 5                   | 0.13     | 0.02                | 0.14       |
| (1,1600) | 1:49:A:LEU:HD13 | 1:52:A:TYR:HD2  | 5                   | 0.13     | 0.02                | 0.14       |
| (2,74)   | 1:79:A:HIS:N    | 1:75:A:LEU:O    | 5                   | 0.13     | 0.01                | 0.13       |
| (1,13)   | 1:19:A:GLU:HG2  | 1:22:A:HIS:H    | 5                   | 0.13     | 0.02                | 0.12       |
| (1,13)   | 1:19:A:GLU:HG3  | 1:22:A:HIS:H    | 5                   | 0.13     | 0.02                | 0.12       |
| (1,916)  | 1:31:A:LEU:HG   | 1:67:A:PHE:H    | 4                   | 0.2      | 0.08                | 0.19       |
| (1,964)  | 2:84:A:PNS:H282 | 1:40:A:MET:HG2  | 4                   | 0.14     | 0.02                | 0.15       |
| (1,964)  | 2:84:A:PNS:H282 | 1:40:A:MET:HG3  | 4                   | 0.14     | 0.02                | 0.15       |
| (1,41)   | 1:1:A:MET:HG2   | 1:4:A:LEU:H     | 4                   | 0.14     | 0.03                | 0.14       |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD11 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD12 | 4                   | 0.13     | 0.02                | 0.12       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD13 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD21 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD22 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD23 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD11 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD12 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD13 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD21 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD22 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD23 | 4                   | 0.13     | 0.02                | 0.12       |
| (2,53)   | 1:51:A:GLU:H    | 1:47:A:THR:O    | 4                   | 0.12     | 0.01                | 0.12       |
| (2,57)   | 1:53:A:PHE:H    | 1:49:A:LEU:O    | 4                   | 0.12     | 0.01                | 0.12       |
| (2,35)   | 1:10:A:ILE:H    | 1:6:A:ALA:O     | 4                   | 0.11     | 0.0                 | 0.11       |
| (2,62)   | 1:73:A:LEU:N    | 1:69:A:THR:O    | 4                   | 0.11     | 0.01                | 0.11       |
| (2,21)   | 1:50:A:GLU:O    | 1:54:A:ASP:N    | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,1979) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG21 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1979) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG22 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1979) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG23 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1979) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG21 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1979) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG22 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1979) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG23 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1979) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG21 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1979) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG22 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1979) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG23 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1992) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG21 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1992) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG22 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1992) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG23 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1992) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG21 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1992) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG22 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1992) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG23 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1992) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG21 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1992) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG22 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1992) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG23 | 3                   | 0.15     | 0.02                | 0.16       |
| (1,1092) | 1:55:A:PHE:HE1  | 1:57:A:VAL:HB   | 3                   | 0.15     | 0.04                | 0.17       |
| (1,1092) | 1:55:A:PHE:HE2  | 1:57:A:VAL:HB   | 3                   | 0.15     | 0.04                | 0.17       |
| (1,1681) | 1:53:A:PHE:H    | 1:55:A:PHE:HD1  | 3                   | 0.15     | 0.03                | 0.15       |
| (1,1681) | 1:53:A:PHE:H    | 1:55:A:PHE:HD2  | 3                   | 0.15     | 0.03                | 0.15       |
| (1,1091) | 1:50:A:GLU:HG2  | 1:57:A:VAL:HB   | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1091) | 1:50:A:GLU:HG3  | 1:57:A:VAL:HB   | 3                   | 0.13     | 0.01                | 0.13       |
| (1,366)  | 1:11:A:LEU:HA   | 1:14:A:VAL:H    | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,400)  | 1:5:A:GLU:HG2   | 1:6:A:ALA:H     | 3                   | 0.12     | 0.02                | 0.12       |
| (1,400)  | 1:5:A:GLU:HG3   | 1:6:A:ALA:H     | 3                   | 0.12     | 0.02                | 0.12       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1977) | 2:84:A:PNS:H311 | 1:40:A:MET:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1977) | 2:84:A:PNS:H312 | 1:40:A:MET:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1977) | 2:84:A:PNS:H313 | 1:40:A:MET:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1990) | 2:84:A:PNS:H311 | 1:40:A:MET:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1990) | 2:84:A:PNS:H312 | 1:40:A:MET:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1990) | 2:84:A:PNS:H313 | 1:40:A:MET:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (1,164)  | 1:30:A:LEU:H    | 1:69:A:THR:HB   | 3                   | 0.11     | 0.01                | 0.11       |
| (1,12)   | 1:2:A:GLN:H     | 1:5:A:GLU:H     | 3                   | 0.11     | 0.01                | 0.11       |
| (2,91)   | 1:66:A:THR:H    | 1:63:A:SER:O    | 3                   | 0.11     | 0.01                | 0.1        |
| (1,847)  | 1:21:A:LYS:HD2  | 1:22:A:HIS:HA   | 2                   | 0.19     | 0.01                | 0.19       |
| (1,225)  | 1:9:A:ASN:H     | 1:21:A:LYS:HE2  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,225)  | 1:9:A:ASN:H     | 1:21:A:LYS:HE3  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,676)  | 1:1:A:MET:HA    | 1:4:A:LEU:H     | 2                   | 0.14     | 0.01                | 0.14       |
| (1,971)  | 1:41:A:ALA:HA   | 1:44:A:ASN:HD22 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1666) | 1:55:A:PHE:HZ   | 1:57:A:VAL:HB   | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,1048) | 1:44:A:ASN:HB3  | 1:48:A:ALA:HB1  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1048) | 1:44:A:ASN:HB3  | 1:48:A:ALA:HB2  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1048) | 1:44:A:ASN:HB3  | 1:48:A:ALA:HB3  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1139) | 1:66:A:THR:HG21 | 1:76:A:PHE:HB2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1139) | 1:66:A:THR:HG22 | 1:76:A:PHE:HB2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1139) | 1:66:A:THR:HG23 | 1:76:A:PHE:HB2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1892) | 1:30:A:LEU:HD11 | 1:68:A:GLU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1892) | 1:30:A:LEU:HD12 | 1:68:A:GLU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1892) | 1:30:A:LEU:HD13 | 1:68:A:GLU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1892) | 1:30:A:LEU:HD21 | 1:68:A:GLU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1892) | 1:30:A:LEU:HD22 | 1:68:A:GLU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1892) | 1:30:A:LEU:HD23 | 1:68:A:GLU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,45)   | 2:84:A:PNS:H281 | 1:40:A:MET:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (2,67)   | 1:76:A:PHE:H    | 1:72:A:SER:O    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,181)  | 1:2:A:GLN:HA    | 1:5:A:GLU:H     | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1889) | 1:30:A:LEU:HD11 | 1:67:A:PHE:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1889) | 1:30:A:LEU:HD12 | 1:67:A:PHE:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1889) | 1:30:A:LEU:HD13 | 1:67:A:PHE:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1889) | 1:30:A:LEU:HD21 | 1:67:A:PHE:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1889) | 1:30:A:LEU:HD22 | 1:67:A:PHE:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1889) | 1:30:A:LEU:HD23 | 1:67:A:PHE:HB2  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1208) | 1:57:A:VAL:HG21 | 1:77:A:VAL:HA   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1208) | 1:57:A:VAL:HG22 | 1:77:A:VAL:HA   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1208) | 1:57:A:VAL:HG23 | 1:77:A:VAL:HA   | 2                   | 0.11     | 0.01                | 0.11       |
| (2,12)   | 1:41:A:ALA:O    | 1:45:A:VAL:H    | 2                   | 0.11     | 0.0                 | 0.11       |
| (2,51)   | 1:50:A:GLU:H    | 1:46:A:ILE:O    | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1019) | 1:9:A:ASN:HD21  | 1:10:A:ILE:HA   | 2                   | 0.11     | 0.0                 | 0.11       |

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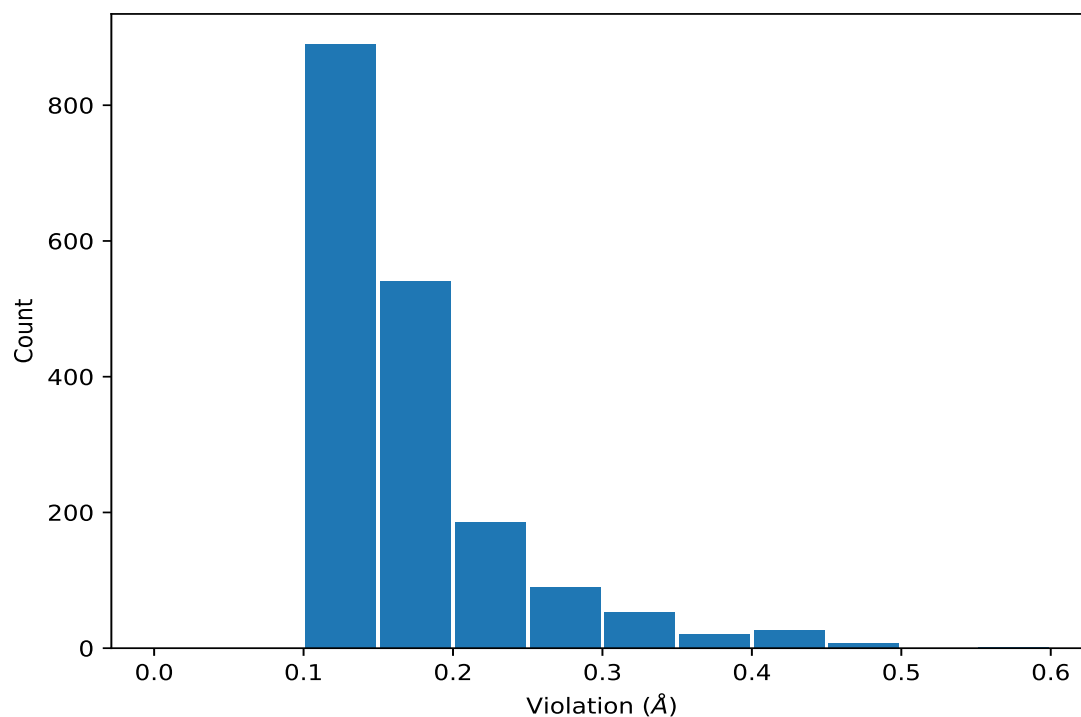
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1994) | 2:84:A:PNS:H371 | 1:46:A:ILE:HD11 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1994) | 2:84:A:PNS:H371 | 1:46:A:ILE:HD12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1994) | 2:84:A:PNS:H371 | 1:46:A:ILE:HD13 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1994) | 2:84:A:PNS:H372 | 1:46:A:ILE:HD11 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1994) | 2:84:A:PNS:H372 | 1:46:A:ILE:HD12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1994) | 2:84:A:PNS:H372 | 1:46:A:ILE:HD13 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,439)  | 1:31:A:LEU:H    | 1:31:A:LEU:HB3  | 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) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 11       | 0.56          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 11       | 0.56          |
| (1,75)   | 1:16:A:ASN:H    | 1:16:A:ASN:HD21 | 14       | 0.47          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 8        | 0.45          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 8        | 0.45          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 12       | 0.45          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 12       | 0.45          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 18       | 0.45          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 18       | 0.45          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 4        | 0.44          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 4        | 0.44          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 10       | 0.44          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 10       | 0.44          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 14       | 0.44          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 14       | 0.44          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 20       | 0.44          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 20       | 0.44          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 9        | 0.43          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 19       | 0.43          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 3        | 0.43          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 3        | 0.43          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 5        | 0.43          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 5        | 0.43          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 17       | 0.43          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 17       | 0.43          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 19       | 0.43          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 19       | 0.43          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 6        | 0.42          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 6        | 0.42          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 20       | 0.41          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 16       | 0.41          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 16       | 0.41          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 16       | 0.4           |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 15       | 0.4           |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 15       | 0.4           |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 1        | 0.39          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 14       | 0.39          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 17       | 0.39          |
| (1,22)   | 1:55:A:PHE:HD1  | 1:58:A:ASP:H    | 9        | 0.39          |
| (1,22)   | 1:55:A:PHE:HD2  | 1:58:A:ASP:H    | 9        | 0.39          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 14       | 0.38          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 14       | 0.38          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 14       | 0.38          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 14       | 0.38          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 14       | 0.38          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 14       | 0.38          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 14       | 0.38          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 14       | 0.38          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 14       | 0.38          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 12       | 0.37          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 15       | 0.37          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 18       | 0.37          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 2        | 0.36          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 2        | 0.36          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 1        | 0.35          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 1        | 0.35          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 8        | 0.34          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG11 | 4        | 0.34          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG12 | 4        | 0.34          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG13 | 4        | 0.34          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG11 | 4        | 0.34          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG12 | 4        | 0.34          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG13 | 4        | 0.34          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 11       | 0.33          |
| (1,1711) | 1:2:A:GLN:HG2   | 1:3:A:HIS:HA    | 1        | 0.33          |
| (1,1711) | 1:2:A:GLN:HG3   | 1:3:A:HIS:HA    | 1        | 0.33          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 2        | 0.32          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 13       | 0.32          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 19       | 0.32          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 19       | 0.32          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 19       | 0.32          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 19       | 0.32          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 19       | 0.32          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 19       | 0.32          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 19       | 0.32          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 19       | 0.32          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 19       | 0.32          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 4        | 0.31          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG21 | 9        | 0.31          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG22 | 9        | 0.31          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG23 | 9        | 0.31          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG21 | 9        | 0.31          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG22 | 9        | 0.31          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG23 | 9        | 0.31          |
| (1,1088) | 1:56:A:SER:HA   | 1:57:A:VAL:HG21 | 7        | 0.31          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1088) | 1:56:A:SER:HA   | 1:57:A:VAL:HG22 | 7        | 0.31          |
| (1,1088) | 1:56:A:SER:HA   | 1:57:A:VAL:HG23 | 7        | 0.31          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 3        | 0.31          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 3        | 0.31          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 3        | 0.31          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 12       | 0.31          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 12       | 0.31          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 12       | 0.31          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 12       | 0.31          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 12       | 0.31          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 12       | 0.31          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 12       | 0.31          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 12       | 0.31          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 12       | 0.31          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 10       | 0.3           |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG11 | 10       | 0.3           |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG12 | 10       | 0.3           |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG13 | 10       | 0.3           |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG11 | 10       | 0.3           |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG12 | 10       | 0.3           |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG13 | 10       | 0.3           |
| (1,1657) | 1:54:A:ASP:HA   | 1:55:A:PHE:HD1  | 8        | 0.3           |
| (1,1657) | 1:54:A:ASP:HA   | 1:55:A:PHE:HD2  | 8        | 0.3           |
| (1,916)  | 1:31:A:LEU:HG   | 1:67:A:PHE:H    | 5        | 0.3           |
| (1,1711) | 1:2:A:GLN:HG2   | 1:3:A:HIS:HA    | 2        | 0.29          |
| (1,1711) | 1:2:A:GLN:HG3   | 1:3:A:HIS:HA    | 2        | 0.29          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 5        | 0.28          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 9        | 0.28          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 16       | 0.28          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 19       | 0.28          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 7        | 0.28          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 7        | 0.28          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 7        | 0.28          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 7        | 0.28          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 7        | 0.28          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 7        | 0.28          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 7        | 0.28          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 7        | 0.28          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 7        | 0.28          |
| (1,741)  | 1:8:A:ARG:HG3   | 1:9:A:ASN:HA    | 9        | 0.28          |
| (1,256)  | 1:1:A:MET:HG3   | 1:4:A:LEU:H     | 10       | 0.28          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG21  | 16       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG22  | 16       | 0.28          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG23  | 16       | 0.28          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 7        | 0.27          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 20       | 0.27          |
| (1,1711) | 1:2:A:GLN:HG2   | 1:3:A:HIS:HA    | 10       | 0.27          |
| (1,1711) | 1:2:A:GLN:HG3   | 1:3:A:HIS:HA    | 10       | 0.27          |
| (1,1711) | 1:2:A:GLN:HG2   | 1:3:A:HIS:HA    | 12       | 0.27          |
| (1,1711) | 1:2:A:GLN:HG3   | 1:3:A:HIS:HA    | 12       | 0.27          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 5        | 0.27          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 5        | 0.27          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 5        | 0.27          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 8        | 0.27          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 8        | 0.27          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 8        | 0.27          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 9        | 0.27          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 9        | 0.27          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 9        | 0.27          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 9        | 0.27          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 9        | 0.27          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 9        | 0.27          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 9        | 0.27          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 9        | 0.27          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 9        | 0.27          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 16       | 0.27          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 16       | 0.27          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 16       | 0.27          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 16       | 0.27          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 16       | 0.27          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 16       | 0.27          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 16       | 0.27          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 16       | 0.27          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 16       | 0.27          |
| (1,833)  | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 20       | 0.27          |
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 7        | 0.27          |
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 7        | 0.27          |
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 7        | 0.27          |
| (1,22)   | 1:55:A:PHE:HD1  | 1:58:A:ASP:H    | 10       | 0.27          |
| (1,22)   | 1:55:A:PHE:HD2  | 1:58:A:ASP:H    | 10       | 0.27          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 14       | 0.26          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 17       | 0.26          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG21 | 17       | 0.26          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG22 | 17       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG23 | 17       | 0.26          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG21 | 17       | 0.26          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG22 | 17       | 0.26          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG23 | 17       | 0.26          |
| (1,1711) | 1:2:A:GLN:HG2   | 1:3:A:HIS:HA    | 5        | 0.26          |
| (1,1711) | 1:2:A:GLN:HG3   | 1:3:A:HIS:HA    | 5        | 0.26          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 13       | 0.26          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 13       | 0.26          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 13       | 0.26          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 17       | 0.26          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 17       | 0.26          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 17       | 0.26          |
| (1,75)   | 1:16:A:ASN:H    | 1:16:A:ASN:HD21 | 16       | 0.26          |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG2   | 13       | 0.25          |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG3   | 13       | 0.25          |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG2   | 13       | 0.25          |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG3   | 13       | 0.25          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 12       | 0.25          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 12       | 0.25          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 12       | 0.25          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 16       | 0.25          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 16       | 0.25          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 16       | 0.25          |
| (1,916)  | 1:31:A:LEU:HG   | 1:67:A:PHE:H    | 12       | 0.25          |
| (1,22)   | 1:55:A:PHE:HD1  | 1:58:A:ASP:H    | 6        | 0.25          |
| (1,22)   | 1:55:A:PHE:HD2  | 1:58:A:ASP:H    | 6        | 0.25          |
| (1,22)   | 1:55:A:PHE:HD1  | 1:58:A:ASP:H    | 8        | 0.25          |
| (1,22)   | 1:55:A:PHE:HD2  | 1:58:A:ASP:H    | 8        | 0.25          |
| (1,7)    | 1:2:A:GLN:HE21  | 1:4:A:LEU:H     | 15       | 0.25          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 6        | 0.24          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 18       | 0.24          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG11 | 11       | 0.24          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG12 | 11       | 0.24          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG13 | 11       | 0.24          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG11 | 11       | 0.24          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG12 | 11       | 0.24          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG13 | 11       | 0.24          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB1  | 14       | 0.24          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB2  | 14       | 0.24          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB3  | 14       | 0.24          |
| (1,1161) | 1:68:A:GLU:HG3  | 1:69:A:THR:HG21 | 12       | 0.24          |
| (1,1161) | 1:68:A:GLU:HG3  | 1:69:A:THR:HG22 | 12       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1161) | 1:68:A:GLU:HG3  | 1:69:A:THR:HG23 | 12       | 0.24          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 7        | 0.24          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 7        | 0.24          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 7        | 0.24          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 15       | 0.24          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 15       | 0.24          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 15       | 0.24          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 15       | 0.24          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 15       | 0.24          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 15       | 0.24          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 15       | 0.24          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 15       | 0.24          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 15       | 0.24          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 17       | 0.24          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 17       | 0.24          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 17       | 0.24          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 17       | 0.24          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 17       | 0.24          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 17       | 0.24          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 17       | 0.24          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 17       | 0.24          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 17       | 0.24          |
| (1,75)   | 1:16:A:ASN:H    | 1:16:A:ASN:HD21 | 4        | 0.24          |
| (2,78)   | 1:43:A:VAL:N    | 1:39:A:SER:O    | 3        | 0.23          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 1        | 0.23          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 12       | 0.23          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 15       | 0.23          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE2  | 7        | 0.23          |
| (1,1369) | 1:21:A:LYS:HA   | 1:21:A:LYS:HE3  | 7        | 0.23          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB1  | 10       | 0.23          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB2  | 10       | 0.23          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB3  | 10       | 0.23          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 20       | 0.23          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 20       | 0.23          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 20       | 0.23          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 20       | 0.23          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 20       | 0.23          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 20       | 0.23          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 20       | 0.23          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 20       | 0.23          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 20       | 0.23          |
| (1,833)  | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 5        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 18       | 0.23          |
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 18       | 0.23          |
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 18       | 0.23          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG11 | 2        | 0.22          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG12 | 2        | 0.22          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG13 | 2        | 0.22          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG11 | 2        | 0.22          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG12 | 2        | 0.22          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG13 | 2        | 0.22          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD11 | 3        | 0.22          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD12 | 3        | 0.22          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD13 | 3        | 0.22          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD21 | 3        | 0.22          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD22 | 3        | 0.22          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD23 | 3        | 0.22          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB1  | 2        | 0.22          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB2  | 2        | 0.22          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB3  | 2        | 0.22          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 4        | 0.22          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 4        | 0.22          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 4        | 0.22          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 11       | 0.22          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 11       | 0.22          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 11       | 0.22          |
| (1,915)  | 1:30:A:LEU:HB2  | 1:31:A:LEU:HG   | 5        | 0.22          |
| (1,456)  | 1:34:A:ILE:HB   | 1:36:A:GLU:H    | 10       | 0.22          |
| (1,94)   | 1:29:A:VAL:H    | 1:69:A:THR:HB   | 12       | 0.22          |
| (1,75)   | 1:16:A:ASN:H    | 1:16:A:ASN:HD21 | 20       | 0.22          |
| (1,7)    | 1:2:A:GLN:HE21  | 1:4:A:LEU:H     | 14       | 0.22          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 2        | 0.21          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 8        | 0.21          |
| (2,2)    | 1:3:A:HIS:O     | 1:7:A:VAL:N     | 5        | 0.21          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 3        | 0.21          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 3        | 0.21          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 3        | 0.21          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 3        | 0.21          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 3        | 0.21          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 3        | 0.21          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 3        | 0.21          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 3        | 0.21          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 3        | 0.21          |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 3        | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 3        | 0.21          |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 3        | 0.21          |
| (1,1711) | 1:2:A:GLN:HG2   | 1:3:A:HIS:HA    | 7        | 0.21          |
| (1,1711) | 1:2:A:GLN:HG3   | 1:3:A:HIS:HA    | 7        | 0.21          |
| (1,1644) | 1:78:A:GLU:HB2  | 1:79:A:HIS:HD2  | 1        | 0.21          |
| (1,1644) | 1:78:A:GLU:HB3  | 1:79:A:HIS:HD2  | 1        | 0.21          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB1  | 9        | 0.21          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB2  | 9        | 0.21          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB3  | 9        | 0.21          |
| (1,1021) | 1:45:A:VAL:HB   | 1:46:A:ILE:HG13 | 8        | 0.21          |
| (1,1021) | 1:45:A:VAL:HB   | 1:46:A:ILE:HG13 | 16       | 0.21          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 9        | 0.21          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 9        | 0.21          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 9        | 0.21          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 15       | 0.21          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 15       | 0.21          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 15       | 0.21          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 20       | 0.21          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 20       | 0.21          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 20       | 0.21          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 4        | 0.21          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 4        | 0.21          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 4        | 0.21          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 4        | 0.21          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 4        | 0.21          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 4        | 0.21          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 4        | 0.21          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 4        | 0.21          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 4        | 0.21          |
| (1,833)  | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 6        | 0.21          |
| (1,741)  | 1:8:A:ARG:HG3   | 1:9:A:ASN:HA    | 11       | 0.21          |
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 2        | 0.21          |
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 2        | 0.21          |
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 2        | 0.21          |
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 10       | 0.21          |
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 10       | 0.21          |
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 10       | 0.21          |
| (1,44)   | 1:40:A:MET:HB3  | 1:43:A:VAL:H    | 7        | 0.21          |
| (1,7)    | 1:2:A:GLN:HE21  | 1:4:A:LEU:H     | 18       | 0.21          |
| (2,93)   | 1:67:A:PHE:H    | 1:64:A:ALA:O    | 11       | 0.2           |
| (2,81)   | 1:13:A:ASP:H    | 1:9:A:ASN:O     | 10       | 0.2           |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 4        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 11       | 0.2           |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 13       | 0.2           |
| (2,73)   | 1:79:A:HIS:H    | 1:75:A:LEU:O    | 20       | 0.2           |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG21 | 11       | 0.2           |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG22 | 11       | 0.2           |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG23 | 11       | 0.2           |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG21 | 11       | 0.2           |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG22 | 11       | 0.2           |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG23 | 11       | 0.2           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD11 | 2        | 0.2           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD12 | 2        | 0.2           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD13 | 2        | 0.2           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD21 | 2        | 0.2           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD22 | 2        | 0.2           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD23 | 2        | 0.2           |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG2   | 9        | 0.2           |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG3   | 9        | 0.2           |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG2   | 9        | 0.2           |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG3   | 9        | 0.2           |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG2   | 10       | 0.2           |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG3   | 10       | 0.2           |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG2   | 10       | 0.2           |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG3   | 10       | 0.2           |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB1  | 6        | 0.2           |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB2  | 6        | 0.2           |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB3  | 6        | 0.2           |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 6        | 0.2           |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 6        | 0.2           |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 6        | 0.2           |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 11       | 0.2           |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 11       | 0.2           |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 11       | 0.2           |
| (1,965)  | 2:84:A:PNS:H281 | 1:40:A:MET:HB2  | 2        | 0.2           |
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 9        | 0.2           |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 9        | 0.2           |
| (1,933)  | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3  | 9        | 0.2           |
| (1,847)  | 1:21:A:LYS:HD2  | 1:22:A:HIS:HA   | 7        | 0.2           |
| (1,833)  | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 4        | 0.2           |
| (1,484)  | 1:57:A:VAL:H    | 1:57:A:VAL:HG21 | 7        | 0.2           |
| (1,484)  | 1:57:A:VAL:H    | 1:57:A:VAL:HG22 | 7        | 0.2           |
| (1,484)  | 1:57:A:VAL:H    | 1:57:A:VAL:HG23 | 7        | 0.2           |
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 4        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 4        | 0.2           |
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 4        | 0.2           |
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 11       | 0.2           |
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 11       | 0.2           |
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 11       | 0.2           |
| (2,73)   | 1:79:A:HIS:H    | 1:75:A:LEU:O    | 2        | 0.19          |
| (2,73)   | 1:79:A:HIS:H    | 1:75:A:LEU:O    | 16       | 0.19          |
| (2,43)   | 1:46:A:ILE:H    | 1:42:A:VAL:O    | 10       | 0.19          |
| (2,28)   | 1:76:A:PHE:O    | 1:80:A:LYS:N    | 17       | 0.19          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG21 | 12       | 0.19          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG22 | 12       | 0.19          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG23 | 12       | 0.19          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG21 | 12       | 0.19          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG22 | 12       | 0.19          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG23 | 12       | 0.19          |
| (1,1681) | 1:53:A:PHE:H    | 1:55:A:PHE:HD1  | 6        | 0.19          |
| (1,1681) | 1:53:A:PHE:H    | 1:55:A:PHE:HD2  | 6        | 0.19          |
| (1,1553) | 1:73:A:LEU:H    | 1:73:A:LEU:HD11 | 7        | 0.19          |
| (1,1553) | 1:73:A:LEU:H    | 1:73:A:LEU:HD12 | 7        | 0.19          |
| (1,1553) | 1:73:A:LEU:H    | 1:73:A:LEU:HD13 | 7        | 0.19          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB1  | 3        | 0.19          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB2  | 3        | 0.19          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB3  | 3        | 0.19          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB1  | 5        | 0.19          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB2  | 5        | 0.19          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB3  | 5        | 0.19          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB1  | 15       | 0.19          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB2  | 15       | 0.19          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB3  | 15       | 0.19          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 7        | 0.19          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 7        | 0.19          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 7        | 0.19          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 3        | 0.19          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 3        | 0.19          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 3        | 0.19          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 3        | 0.19          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 3        | 0.19          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 3        | 0.19          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 3        | 0.19          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 3        | 0.19          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 3        | 0.19          |
| (1,741)  | 1:8:A:ARG:HG3   | 1:9:A:ASN:HA    | 14       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,299)  | 1:13:A:ASP:HA   | 1:15:A:LEU:H    | 11       | 0.19          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG21  | 19       | 0.19          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG22  | 19       | 0.19          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG23  | 19       | 0.19          |
| (1,22)   | 1:55:A:PHE:HD1  | 1:58:A:ASP:H    | 15       | 0.19          |
| (1,22)   | 1:55:A:PHE:HD2  | 1:58:A:ASP:H    | 15       | 0.19          |
| (2,81)   | 1:13:A:ASP:H    | 1:9:A:ASN:O     | 12       | 0.18          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 10       | 0.18          |
| (2,73)   | 1:79:A:HIS:H    | 1:75:A:LEU:O    | 4        | 0.18          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 1        | 0.18          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 11       | 0.18          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 16       | 0.18          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG21 | 14       | 0.18          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG22 | 14       | 0.18          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG23 | 14       | 0.18          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG21 | 14       | 0.18          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG22 | 14       | 0.18          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG23 | 14       | 0.18          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 10       | 0.18          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 10       | 0.18          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 10       | 0.18          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 10       | 0.18          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 10       | 0.18          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 10       | 0.18          |
| (1,1388) | 1:24:A:LEU:HD11 | 1:25:A:THR:HA   | 8        | 0.18          |
| (1,1388) | 1:24:A:LEU:HD12 | 1:25:A:THR:HA   | 8        | 0.18          |
| (1,1388) | 1:24:A:LEU:HD13 | 1:25:A:THR:HA   | 8        | 0.18          |
| (1,1092) | 1:55:A:PHE:HE1  | 1:57:A:VAL:HB   | 18       | 0.18          |
| (1,1092) | 1:55:A:PHE:HE2  | 1:57:A:VAL:HB   | 18       | 0.18          |
| (1,1021) | 1:45:A:VAL:HB   | 1:46:A:ILE:HG13 | 4        | 0.18          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 13       | 0.18          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 13       | 0.18          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 13       | 0.18          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 2        | 0.18          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 2        | 0.18          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 2        | 0.18          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 14       | 0.18          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 14       | 0.18          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 14       | 0.18          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 2        | 0.18          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 2        | 0.18          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 2        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 2        | 0.18          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 2        | 0.18          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 2        | 0.18          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 2        | 0.18          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 2        | 0.18          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 2        | 0.18          |
| (1,847)  | 1:21:A:LYS:HD2  | 1:22:A:HIS:HA   | 9        | 0.18          |
| (1,772)  | 1:10:A:ILE:HG21 | 1:13:A:ASP:HB2  | 1        | 0.18          |
| (1,772)  | 1:10:A:ILE:HG22 | 1:13:A:ASP:HB2  | 1        | 0.18          |
| (1,772)  | 1:10:A:ILE:HG23 | 1:13:A:ASP:HB2  | 1        | 0.18          |
| (1,741)  | 1:8:A:ARG:HG3   | 1:9:A:ASN:HA    | 7        | 0.18          |
| (1,554)  | 1:32:A:GLY:H    | 1:37:A:LEU:HG   | 16       | 0.18          |
| (1,537)  | 1:69:A:THR:H    | 1:69:A:THR:HG21 | 12       | 0.18          |
| (1,537)  | 1:69:A:THR:H    | 1:69:A:THR:HG22 | 12       | 0.18          |
| (1,537)  | 1:69:A:THR:H    | 1:69:A:THR:HG23 | 12       | 0.18          |
| (1,456)  | 1:34:A:ILE:HB   | 1:36:A:GLU:H    | 1        | 0.18          |
| (1,456)  | 1:34:A:ILE:HB   | 1:36:A:GLU:H    | 8        | 0.18          |
| (1,456)  | 1:34:A:ILE:HB   | 1:36:A:GLU:H    | 11       | 0.18          |
| (1,44)   | 1:40:A:MET:HB3  | 1:43:A:VAL:H    | 3        | 0.18          |
| (1,44)   | 1:40:A:MET:HB3  | 1:43:A:VAL:H    | 18       | 0.18          |
| (1,41)   | 1:1:A:MET:HG2   | 1:4:A:LEU:H     | 16       | 0.18          |
| (2,81)   | 1:13:A:ASP:H    | 1:9:A:ASN:O     | 1        | 0.17          |
| (2,73)   | 1:79:A:HIS:H    | 1:75:A:LEU:O    | 11       | 0.17          |
| (2,73)   | 1:79:A:HIS:H    | 1:75:A:LEU:O    | 17       | 0.17          |
| (2,61)   | 1:73:A:LEU:H    | 1:69:A:THR:O    | 19       | 0.17          |
| (2,61)   | 1:73:A:LEU:H    | 1:69:A:THR:O    | 20       | 0.17          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 3        | 0.17          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 10       | 0.17          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 19       | 0.17          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG11 | 3        | 0.17          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG12 | 3        | 0.17          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG13 | 3        | 0.17          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG11 | 3        | 0.17          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG12 | 3        | 0.17          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG13 | 3        | 0.17          |
| (1,1992) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG21 | 18       | 0.17          |
| (1,1992) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG22 | 18       | 0.17          |
| (1,1992) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG23 | 18       | 0.17          |
| (1,1992) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG21 | 18       | 0.17          |
| (1,1992) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG22 | 18       | 0.17          |
| (1,1992) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG23 | 18       | 0.17          |
| (1,1992) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG21 | 18       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1992) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG22 | 18       | 0.17          |
| (1,1992) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG23 | 18       | 0.17          |
| (1,1979) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG21 | 18       | 0.17          |
| (1,1979) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG22 | 18       | 0.17          |
| (1,1979) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG23 | 18       | 0.17          |
| (1,1979) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG21 | 18       | 0.17          |
| (1,1979) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG22 | 18       | 0.17          |
| (1,1979) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG23 | 18       | 0.17          |
| (1,1979) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG21 | 18       | 0.17          |
| (1,1979) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG22 | 18       | 0.17          |
| (1,1979) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG23 | 18       | 0.17          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD11 | 3        | 0.17          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD12 | 3        | 0.17          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD13 | 3        | 0.17          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD21 | 3        | 0.17          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD22 | 3        | 0.17          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD23 | 3        | 0.17          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD11 | 3        | 0.17          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD12 | 3        | 0.17          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD13 | 3        | 0.17          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD21 | 3        | 0.17          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD22 | 3        | 0.17          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD23 | 3        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 2        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 2        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 2        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 2        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 2        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 2        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 4        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 4        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 4        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 4        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 4        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 4        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 5        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 5        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 5        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 5        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 5        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 5        | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 20       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 20       | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 20       | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 20       | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 20       | 0.17          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 20       | 0.17          |
| (1,1782) | 1:13:A:ASP:HB3  | 1:14:A:VAL:HG11 | 5        | 0.17          |
| (1,1782) | 1:13:A:ASP:HB3  | 1:14:A:VAL:HG12 | 5        | 0.17          |
| (1,1782) | 1:13:A:ASP:HB3  | 1:14:A:VAL:HG13 | 5        | 0.17          |
| (1,1782) | 1:13:A:ASP:HB3  | 1:14:A:VAL:HG21 | 5        | 0.17          |
| (1,1782) | 1:13:A:ASP:HB3  | 1:14:A:VAL:HG22 | 5        | 0.17          |
| (1,1782) | 1:13:A:ASP:HB3  | 1:14:A:VAL:HG23 | 5        | 0.17          |
| (1,1722) | 1:4:A:LEU:HD11  | 1:5:A:GLU:HA    | 5        | 0.17          |
| (1,1722) | 1:4:A:LEU:HD12  | 1:5:A:GLU:HA    | 5        | 0.17          |
| (1,1722) | 1:4:A:LEU:HD13  | 1:5:A:GLU:HA    | 5        | 0.17          |
| (1,1722) | 1:4:A:LEU:HD21  | 1:5:A:GLU:HA    | 5        | 0.17          |
| (1,1722) | 1:4:A:LEU:HD22  | 1:5:A:GLU:HA    | 5        | 0.17          |
| (1,1722) | 1:4:A:LEU:HD23  | 1:5:A:GLU:HA    | 5        | 0.17          |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG2   | 2        | 0.17          |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG3   | 2        | 0.17          |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG2   | 2        | 0.17          |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG3   | 2        | 0.17          |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG2   | 17       | 0.17          |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG3   | 17       | 0.17          |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG2   | 17       | 0.17          |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG3   | 17       | 0.17          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB1  | 12       | 0.17          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB2  | 12       | 0.17          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB3  | 12       | 0.17          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD11 | 14       | 0.17          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD12 | 14       | 0.17          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD13 | 14       | 0.17          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD11 | 14       | 0.17          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD12 | 14       | 0.17          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD13 | 14       | 0.17          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD11 | 14       | 0.17          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD12 | 14       | 0.17          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD13 | 14       | 0.17          |
| (1,1092) | 1:55:A:PHE:HE1  | 1:57:A:VAL:HB   | 2        | 0.17          |
| (1,1092) | 1:55:A:PHE:HE2  | 1:57:A:VAL:HB   | 2        | 0.17          |
| (1,1021) | 1:45:A:VAL:HB   | 1:46:A:ILE:HG13 | 15       | 0.17          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 1        | 0.17          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 1        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 1        | 0.17          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 10       | 0.17          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 10       | 0.17          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 10       | 0.17          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 5        | 0.17          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 5        | 0.17          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 5        | 0.17          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 5        | 0.17          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 5        | 0.17          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 5        | 0.17          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 5        | 0.17          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 5        | 0.17          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 5        | 0.17          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 13       | 0.17          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 13       | 0.17          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 13       | 0.17          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 13       | 0.17          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 13       | 0.17          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 13       | 0.17          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 13       | 0.17          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 13       | 0.17          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 13       | 0.17          |
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 19       | 0.17          |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 19       | 0.17          |
| (1,933)  | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3  | 19       | 0.17          |
| (1,741)  | 1:8:A:ARG:HG3   | 1:9:A:ASN:HA    | 13       | 0.17          |
| (1,741)  | 1:8:A:ARG:HG3   | 1:9:A:ASN:HA    | 17       | 0.17          |
| (1,649)  | 1:6:A:ALA:HB1   | 1:9:A:ASN:HD22  | 4        | 0.17          |
| (1,649)  | 1:6:A:ALA:HB2   | 1:9:A:ASN:HD22  | 4        | 0.17          |
| (1,649)  | 1:6:A:ALA:HB3   | 1:9:A:ASN:HD22  | 4        | 0.17          |
| (1,456)  | 1:34:A:ILE:HB   | 1:36:A:GLU:H    | 6        | 0.17          |
| (1,456)  | 1:34:A:ILE:HB   | 1:36:A:GLU:H    | 7        | 0.17          |
| (1,456)  | 1:34:A:ILE:HB   | 1:36:A:GLU:H    | 20       | 0.17          |
| (1,256)  | 1:1:A:MET:HG3   | 1:4:A:LEU:H     | 9        | 0.17          |
| (1,185)  | 1:4:A:LEU:H     | 1:7:A:VAL:HB    | 7        | 0.17          |
| (1,185)  | 1:4:A:LEU:H     | 1:7:A:VAL:HB    | 15       | 0.17          |
| (1,185)  | 1:4:A:LEU:H     | 1:7:A:VAL:HB    | 19       | 0.17          |
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 3        | 0.17          |
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 3        | 0.17          |
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 3        | 0.17          |
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 12       | 0.17          |
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 12       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 12       | 0.17          |
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 17       | 0.17          |
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 17       | 0.17          |
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 17       | 0.17          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG21  | 9        | 0.17          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG22  | 9        | 0.17          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG23  | 9        | 0.17          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG21  | 20       | 0.17          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG22  | 20       | 0.17          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG23  | 20       | 0.17          |
| (1,13)   | 1:19:A:GLU:HG2  | 1:22:A:HIS:H    | 20       | 0.17          |
| (1,13)   | 1:19:A:GLU:HG3  | 1:22:A:HIS:H    | 20       | 0.17          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 7        | 0.16          |
| (2,73)   | 1:79:A:HIS:H    | 1:75:A:LEU:O    | 8        | 0.16          |
| (2,61)   | 1:73:A:LEU:H    | 1:69:A:THR:O    | 9        | 0.16          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 5        | 0.16          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 14       | 0.16          |
| (1,2010) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG21 | 7        | 0.16          |
| (1,2010) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG22 | 7        | 0.16          |
| (1,2010) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG23 | 7        | 0.16          |
| (1,2010) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG21 | 7        | 0.16          |
| (1,2010) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG22 | 7        | 0.16          |
| (1,2010) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG23 | 7        | 0.16          |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG21 | 10       | 0.16          |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG22 | 10       | 0.16          |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG23 | 10       | 0.16          |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG21 | 10       | 0.16          |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG22 | 10       | 0.16          |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG23 | 10       | 0.16          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG21 | 7        | 0.16          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG22 | 7        | 0.16          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG23 | 7        | 0.16          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG21 | 7        | 0.16          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG22 | 7        | 0.16          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG23 | 7        | 0.16          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG21 | 19       | 0.16          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG22 | 19       | 0.16          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG23 | 19       | 0.16          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG21 | 19       | 0.16          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG22 | 19       | 0.16          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG23 | 19       | 0.16          |
| (1,1992) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG21 | 1        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1992) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG22 | 1        | 0.16          |
| (1,1992) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG23 | 1        | 0.16          |
| (1,1992) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG21 | 1        | 0.16          |
| (1,1992) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG22 | 1        | 0.16          |
| (1,1992) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG23 | 1        | 0.16          |
| (1,1992) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG21 | 1        | 0.16          |
| (1,1992) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG22 | 1        | 0.16          |
| (1,1992) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG23 | 1        | 0.16          |
| (1,1979) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG21 | 1        | 0.16          |
| (1,1979) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG22 | 1        | 0.16          |
| (1,1979) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG23 | 1        | 0.16          |
| (1,1979) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG21 | 1        | 0.16          |
| (1,1979) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG22 | 1        | 0.16          |
| (1,1979) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG23 | 1        | 0.16          |
| (1,1979) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG21 | 1        | 0.16          |
| (1,1979) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG22 | 1        | 0.16          |
| (1,1979) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG23 | 1        | 0.16          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 12       | 0.16          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 12       | 0.16          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 12       | 0.16          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 12       | 0.16          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 12       | 0.16          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 12       | 0.16          |
| (1,1722) | 1:4:A:LEU:HD11  | 1:5:A:GLU:HA    | 10       | 0.16          |
| (1,1722) | 1:4:A:LEU:HD12  | 1:5:A:GLU:HA    | 10       | 0.16          |
| (1,1722) | 1:4:A:LEU:HD13  | 1:5:A:GLU:HA    | 10       | 0.16          |
| (1,1722) | 1:4:A:LEU:HD21  | 1:5:A:GLU:HA    | 10       | 0.16          |
| (1,1722) | 1:4:A:LEU:HD22  | 1:5:A:GLU:HA    | 10       | 0.16          |
| (1,1722) | 1:4:A:LEU:HD23  | 1:5:A:GLU:HA    | 10       | 0.16          |
| (1,1722) | 1:4:A:LEU:HD11  | 1:5:A:GLU:HA    | 12       | 0.16          |
| (1,1722) | 1:4:A:LEU:HD12  | 1:5:A:GLU:HA    | 12       | 0.16          |
| (1,1722) | 1:4:A:LEU:HD13  | 1:5:A:GLU:HA    | 12       | 0.16          |
| (1,1722) | 1:4:A:LEU:HD21  | 1:5:A:GLU:HA    | 12       | 0.16          |
| (1,1722) | 1:4:A:LEU:HD22  | 1:5:A:GLU:HA    | 12       | 0.16          |
| (1,1722) | 1:4:A:LEU:HD23  | 1:5:A:GLU:HA    | 12       | 0.16          |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG2   | 5        | 0.16          |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG3   | 5        | 0.16          |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG2   | 5        | 0.16          |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG3   | 5        | 0.16          |
| (1,1600) | 1:49:A:LEU:HD11 | 1:52:A:TYR:HD1  | 9        | 0.16          |
| (1,1600) | 1:49:A:LEU:HD11 | 1:52:A:TYR:HD2  | 9        | 0.16          |
| (1,1600) | 1:49:A:LEU:HD12 | 1:52:A:TYR:HD1  | 9        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1600) | 1:49:A:LEU:HD12 | 1:52:A:TYR:HD2  | 9        | 0.16          |
| (1,1600) | 1:49:A:LEU:HD13 | 1:52:A:TYR:HD1  | 9        | 0.16          |
| (1,1600) | 1:49:A:LEU:HD13 | 1:52:A:TYR:HD2  | 9        | 0.16          |
| (1,1388) | 1:24:A:LEU:HD11 | 1:25:A:THR:HA   | 5        | 0.16          |
| (1,1388) | 1:24:A:LEU:HD12 | 1:25:A:THR:HA   | 5        | 0.16          |
| (1,1388) | 1:24:A:LEU:HD13 | 1:25:A:THR:HA   | 5        | 0.16          |
| (1,1268) | 1:56:A:SER:H    | 1:81:A:LEU:HD11 | 6        | 0.16          |
| (1,1268) | 1:56:A:SER:H    | 1:81:A:LEU:HD12 | 6        | 0.16          |
| (1,1268) | 1:56:A:SER:H    | 1:81:A:LEU:HD13 | 6        | 0.16          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB1  | 17       | 0.16          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB2  | 17       | 0.16          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB3  | 17       | 0.16          |
| (1,1021) | 1:45:A:VAL:HB   | 1:46:A:ILE:HG13 | 17       | 0.16          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 5        | 0.16          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 5        | 0.16          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 5        | 0.16          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 10       | 0.16          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 10       | 0.16          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 10       | 0.16          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 19       | 0.16          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 19       | 0.16          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 19       | 0.16          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 20       | 0.16          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 20       | 0.16          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 20       | 0.16          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 18       | 0.16          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 18       | 0.16          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 18       | 0.16          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG21 | 8        | 0.16          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG22 | 8        | 0.16          |
| (1,984)  | 2:84:A:PNS:H311 | 1:42:A:VAL:HG23 | 8        | 0.16          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG21 | 8        | 0.16          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG22 | 8        | 0.16          |
| (1,984)  | 2:84:A:PNS:H312 | 1:42:A:VAL:HG23 | 8        | 0.16          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG21 | 8        | 0.16          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG22 | 8        | 0.16          |
| (1,984)  | 2:84:A:PNS:H313 | 1:42:A:VAL:HG23 | 8        | 0.16          |
| (1,964)  | 2:84:A:PNS:H282 | 1:40:A:MET:HG2  | 3        | 0.16          |
| (1,964)  | 2:84:A:PNS:H282 | 1:40:A:MET:HG3  | 3        | 0.16          |
| (1,964)  | 2:84:A:PNS:H282 | 1:40:A:MET:HG2  | 18       | 0.16          |
| (1,964)  | 2:84:A:PNS:H282 | 1:40:A:MET:HG3  | 18       | 0.16          |
| (1,833)  | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 3        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,833)  | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 18       | 0.16          |
| (1,772)  | 1:10:A:ILE:HG21 | 1:13:A:ASP:HB2  | 6        | 0.16          |
| (1,772)  | 1:10:A:ILE:HG22 | 1:13:A:ASP:HB2  | 6        | 0.16          |
| (1,772)  | 1:10:A:ILE:HG23 | 1:13:A:ASP:HB2  | 6        | 0.16          |
| (1,741)  | 1:8:A:ARG:HG3   | 1:9:A:ASN:HA    | 3        | 0.16          |
| (1,456)  | 1:34:A:ILE:HB   | 1:36:A:GLU:H    | 5        | 0.16          |
| (1,456)  | 1:34:A:ILE:HB   | 1:36:A:GLU:H    | 15       | 0.16          |
| (1,256)  | 1:1:A:MET:HG3   | 1:4:A:LEU:H     | 2        | 0.16          |
| (1,185)  | 1:4:A:LEU:H     | 1:7:A:VAL:HB    | 16       | 0.16          |
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 5        | 0.16          |
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 5        | 0.16          |
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 5        | 0.16          |
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 14       | 0.16          |
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 14       | 0.16          |
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 14       | 0.16          |
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 15       | 0.16          |
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 15       | 0.16          |
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 15       | 0.16          |
| (1,44)   | 1:40:A:MET:HB3  | 1:43:A:VAL:H    | 10       | 0.16          |
| (1,44)   | 1:40:A:MET:HB3  | 1:43:A:VAL:H    | 13       | 0.16          |
| (1,29)   | 1:2:A:GLN:H     | 1:74:A:ALA:HB1  | 11       | 0.16          |
| (1,29)   | 1:2:A:GLN:H     | 1:74:A:ALA:HB2  | 11       | 0.16          |
| (1,29)   | 1:2:A:GLN:H     | 1:74:A:ALA:HB3  | 11       | 0.16          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG21  | 11       | 0.16          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG22  | 11       | 0.16          |
| (1,25)   | 1:3:A:HIS:H     | 1:7:A:VAL:HG23  | 11       | 0.16          |
| (1,7)    | 1:2:A:GLN:HE21  | 1:4:A:LEU:H     | 20       | 0.16          |
| (2,81)   | 1:13:A:ASP:H    | 1:9:A:ASN:O     | 4        | 0.15          |
| (2,81)   | 1:13:A:ASP:H    | 1:9:A:ASN:O     | 11       | 0.15          |
| (2,81)   | 1:13:A:ASP:H    | 1:9:A:ASN:O     | 17       | 0.15          |
| (2,77)   | 1:43:A:VAL:H    | 1:39:A:SER:O    | 5        | 0.15          |
| (2,75)   | 1:80:A:LYS:H    | 1:76:A:PHE:O    | 11       | 0.15          |
| (2,61)   | 1:73:A:LEU:H    | 1:69:A:THR:O    | 2        | 0.15          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 2        | 0.15          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 4        | 0.15          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 8        | 0.15          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 9        | 0.15          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 15       | 0.15          |
| (2,43)   | 1:46:A:ILE:H    | 1:42:A:VAL:O    | 19       | 0.15          |
| (2,28)   | 1:76:A:PHE:O    | 1:80:A:LYS:N    | 8        | 0.15          |
| (2,28)   | 1:76:A:PHE:O    | 1:80:A:LYS:N    | 18       | 0.15          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG21 | 5        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG22 | 5        | 0.15          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG23 | 5        | 0.15          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG21 | 5        | 0.15          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG22 | 5        | 0.15          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG23 | 5        | 0.15          |
| (1,1943) | 1:37:A:LEU:HD11 | 1:42:A:VAL:HA   | 6        | 0.15          |
| (1,1943) | 1:37:A:LEU:HD12 | 1:42:A:VAL:HA   | 6        | 0.15          |
| (1,1943) | 1:37:A:LEU:HD13 | 1:42:A:VAL:HA   | 6        | 0.15          |
| (1,1943) | 1:37:A:LEU:HD21 | 1:42:A:VAL:HA   | 6        | 0.15          |
| (1,1943) | 1:37:A:LEU:HD22 | 1:42:A:VAL:HA   | 6        | 0.15          |
| (1,1943) | 1:37:A:LEU:HD23 | 1:42:A:VAL:HA   | 6        | 0.15          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 3        | 0.15          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 3        | 0.15          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 3        | 0.15          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 3        | 0.15          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 3        | 0.15          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 3        | 0.15          |
| (1,1822) | 1:15:A:LEU:HD11 | 1:41:A:ALA:HB1  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD11 | 1:41:A:ALA:HB2  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD11 | 1:41:A:ALA:HB3  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD12 | 1:41:A:ALA:HB1  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD12 | 1:41:A:ALA:HB2  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD12 | 1:41:A:ALA:HB3  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD13 | 1:41:A:ALA:HB1  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD13 | 1:41:A:ALA:HB2  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD13 | 1:41:A:ALA:HB3  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD21 | 1:41:A:ALA:HB1  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD21 | 1:41:A:ALA:HB2  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD21 | 1:41:A:ALA:HB3  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD22 | 1:41:A:ALA:HB1  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD22 | 1:41:A:ALA:HB2  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD22 | 1:41:A:ALA:HB3  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD23 | 1:41:A:ALA:HB1  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD23 | 1:41:A:ALA:HB2  | 13       | 0.15          |
| (1,1822) | 1:15:A:LEU:HD23 | 1:41:A:ALA:HB3  | 13       | 0.15          |
| (1,1722) | 1:4:A:LEU:HD11  | 1:5:A:GLU:HA    | 17       | 0.15          |
| (1,1722) | 1:4:A:LEU:HD12  | 1:5:A:GLU:HA    | 17       | 0.15          |
| (1,1722) | 1:4:A:LEU:HD13  | 1:5:A:GLU:HA    | 17       | 0.15          |
| (1,1722) | 1:4:A:LEU:HD21  | 1:5:A:GLU:HA    | 17       | 0.15          |
| (1,1722) | 1:4:A:LEU:HD22  | 1:5:A:GLU:HA    | 17       | 0.15          |
| (1,1722) | 1:4:A:LEU:HD23  | 1:5:A:GLU:HA    | 17       | 0.15          |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG2   | 3        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG3   | 3        | 0.15          |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG2   | 3        | 0.15          |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG3   | 3        | 0.15          |
| (1,1681) | 1:53:A:PHE:H    | 1:55:A:PHE:HD1  | 9        | 0.15          |
| (1,1681) | 1:53:A:PHE:H    | 1:55:A:PHE:HD2  | 9        | 0.15          |
| (1,1388) | 1:24:A:LEU:HD11 | 1:25:A:THR:HA   | 3        | 0.15          |
| (1,1388) | 1:24:A:LEU:HD12 | 1:25:A:THR:HA   | 3        | 0.15          |
| (1,1388) | 1:24:A:LEU:HD13 | 1:25:A:THR:HA   | 3        | 0.15          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB1  | 4        | 0.15          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB2  | 4        | 0.15          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB3  | 4        | 0.15          |
| (1,1118) | 1:57:A:VAL:HB   | 1:62:A:ILE:HD11 | 7        | 0.15          |
| (1,1118) | 1:57:A:VAL:HB   | 1:62:A:ILE:HD12 | 7        | 0.15          |
| (1,1118) | 1:57:A:VAL:HB   | 1:62:A:ILE:HD13 | 7        | 0.15          |
| (1,1048) | 1:44:A:ASN:HB3  | 1:48:A:ALA:HB1  | 6        | 0.15          |
| (1,1048) | 1:44:A:ASN:HB3  | 1:48:A:ALA:HB2  | 6        | 0.15          |
| (1,1048) | 1:44:A:ASN:HB3  | 1:48:A:ALA:HB3  | 6        | 0.15          |
| (1,1021) | 1:45:A:VAL:HB   | 1:46:A:ILE:HG13 | 14       | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 2        | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 2        | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 2        | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 3        | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 3        | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 3        | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 4        | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 4        | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 4        | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 8        | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 8        | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 8        | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 12       | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 12       | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 12       | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 14       | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 14       | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 14       | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 15       | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 15       | 0.15          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 15       | 0.15          |
| (1,971)  | 1:41:A:ALA:HA   | 1:44:A:ASN:HD22 | 1        | 0.15          |
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 1        | 0.15          |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 1        | 0.15          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,933) | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3 | 1        | 0.15          |
| (1,933) | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3 | 4        | 0.15          |
| (1,933) | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3 | 4        | 0.15          |
| (1,933) | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3 | 4        | 0.15          |
| (1,933) | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3 | 5        | 0.15          |
| (1,933) | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3 | 5        | 0.15          |
| (1,933) | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3 | 5        | 0.15          |
| (1,933) | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3 | 10       | 0.15          |
| (1,933) | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3 | 10       | 0.15          |
| (1,933) | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3 | 10       | 0.15          |
| (1,933) | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3 | 13       | 0.15          |
| (1,933) | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3 | 13       | 0.15          |
| (1,933) | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3 | 13       | 0.15          |
| (1,833) | 1:12:A:GLY:H    | 1:21:A:LYS:HG2 | 8        | 0.15          |
| (1,833) | 1:12:A:GLY:H    | 1:21:A:LYS:HG2 | 14       | 0.15          |
| (1,833) | 1:12:A:GLY:H    | 1:21:A:LYS:HG2 | 19       | 0.15          |
| (1,768) | 1:13:A:ASP:HA   | 1:21:A:LYS:HD3 | 13       | 0.15          |
| (1,649) | 1:6:A:ALA:HB1   | 1:9:A:ASN:HD22 | 12       | 0.15          |
| (1,649) | 1:6:A:ALA:HB2   | 1:9:A:ASN:HD22 | 12       | 0.15          |
| (1,649) | 1:6:A:ALA:HB3   | 1:9:A:ASN:HD22 | 12       | 0.15          |
| (1,649) | 1:6:A:ALA:HB1   | 1:9:A:ASN:HD22 | 19       | 0.15          |
| (1,649) | 1:6:A:ALA:HB2   | 1:9:A:ASN:HD22 | 19       | 0.15          |
| (1,649) | 1:6:A:ALA:HB3   | 1:9:A:ASN:HD22 | 19       | 0.15          |
| (1,642) | 1:2:A:GLN:HA    | 1:2:A:GLN:HE21 | 11       | 0.15          |
| (1,456) | 1:34:A:ILE:HB   | 1:36:A:GLU:H   | 14       | 0.15          |
| (1,225) | 1:9:A:ASN:H     | 1:21:A:LYS:HE2 | 1        | 0.15          |
| (1,225) | 1:9:A:ASN:H     | 1:21:A:LYS:HE3 | 1        | 0.15          |
| (1,185) | 1:4:A:LEU:H     | 1:7:A:VAL:HB   | 20       | 0.15          |
| (1,146) | 1:7:A:VAL:HG21  | 1:73:A:LEU:H   | 19       | 0.15          |
| (1,146) | 1:7:A:VAL:HG22  | 1:73:A:LEU:H   | 19       | 0.15          |
| (1,146) | 1:7:A:VAL:HG23  | 1:73:A:LEU:H   | 19       | 0.15          |
| (1,44)  | 1:40:A:MET:HB3  | 1:43:A:VAL:H   | 2        | 0.15          |
| (1,44)  | 1:40:A:MET:HB3  | 1:43:A:VAL:H   | 4        | 0.15          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG21 | 8        | 0.15          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG22 | 8        | 0.15          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG23 | 8        | 0.15          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG21 | 17       | 0.15          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG22 | 17       | 0.15          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG23 | 17       | 0.15          |
| (1,22)  | 1:55:A:PHE:HD1  | 1:58:A:ASP:H   | 1        | 0.15          |
| (1,22)  | 1:55:A:PHE:HD2  | 1:58:A:ASP:H   | 1        | 0.15          |
| (2,93)  | 1:67:A:PHE:H    | 1:64:A:ALA:O   | 18       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,81)   | 1:13:A:ASP:H    | 1:9:A:ASN:O     | 2        | 0.14          |
| (2,81)   | 1:13:A:ASP:H    | 1:9:A:ASN:O     | 18       | 0.14          |
| (2,74)   | 1:79:A:HIS:N    | 1:75:A:LEU:O    | 2        | 0.14          |
| (2,74)   | 1:79:A:HIS:N    | 1:75:A:LEU:O    | 16       | 0.14          |
| (2,61)   | 1:73:A:LEU:H    | 1:69:A:THR:O    | 3        | 0.14          |
| (2,61)   | 1:73:A:LEU:H    | 1:69:A:THR:O    | 7        | 0.14          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 7        | 0.14          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 13       | 0.14          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 17       | 0.14          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 18       | 0.14          |
| (2,59)   | 1:54:A:ASP:H    | 1:50:A:GLU:O    | 20       | 0.14          |
| (2,57)   | 1:53:A:PHE:H    | 1:49:A:LEU:O    | 11       | 0.14          |
| (2,43)   | 1:46:A:ILE:H    | 1:42:A:VAL:O    | 4        | 0.14          |
| (2,43)   | 1:46:A:ILE:H    | 1:42:A:VAL:O    | 9        | 0.14          |
| (2,2)    | 1:3:A:HIS:O     | 1:7:A:VAL:N     | 10       | 0.14          |
| (2,2)    | 1:3:A:HIS:O     | 1:7:A:VAL:N     | 15       | 0.14          |
| (2,1)    | 1:3:A:HIS:O     | 1:7:A:VAL:H     | 12       | 0.14          |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG21 | 16       | 0.14          |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG22 | 16       | 0.14          |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG23 | 16       | 0.14          |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG21 | 16       | 0.14          |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG22 | 16       | 0.14          |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG23 | 16       | 0.14          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG11 | 5        | 0.14          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG12 | 5        | 0.14          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG13 | 5        | 0.14          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG11 | 5        | 0.14          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG12 | 5        | 0.14          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG13 | 5        | 0.14          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG11 | 7        | 0.14          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG12 | 7        | 0.14          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG13 | 7        | 0.14          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG11 | 7        | 0.14          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG12 | 7        | 0.14          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG13 | 7        | 0.14          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG11 | 13       | 0.14          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG12 | 13       | 0.14          |
| (1,1995) | 2:84:A:PNS:H381 | 1:42:A:VAL:HG13 | 13       | 0.14          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG11 | 13       | 0.14          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG12 | 13       | 0.14          |
| (1,1995) | 2:84:A:PNS:H382 | 1:42:A:VAL:HG13 | 13       | 0.14          |
| (1,1941) | 1:37:A:LEU:HD11 | 1:38:A:ASP:H    | 6        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1941) | 1:37:A:LEU:HD12 | 1:38:A:ASP:H    | 6        | 0.14          |
| (1,1941) | 1:37:A:LEU:HD13 | 1:38:A:ASP:H    | 6        | 0.14          |
| (1,1941) | 1:37:A:LEU:HD21 | 1:38:A:ASP:H    | 6        | 0.14          |
| (1,1941) | 1:37:A:LEU:HD22 | 1:38:A:ASP:H    | 6        | 0.14          |
| (1,1941) | 1:37:A:LEU:HD23 | 1:38:A:ASP:H    | 6        | 0.14          |
| (1,1892) | 1:30:A:LEU:HD11 | 1:68:A:GLU:H    | 14       | 0.14          |
| (1,1892) | 1:30:A:LEU:HD12 | 1:68:A:GLU:H    | 14       | 0.14          |
| (1,1892) | 1:30:A:LEU:HD13 | 1:68:A:GLU:H    | 14       | 0.14          |
| (1,1892) | 1:30:A:LEU:HD21 | 1:68:A:GLU:H    | 14       | 0.14          |
| (1,1892) | 1:30:A:LEU:HD22 | 1:68:A:GLU:H    | 14       | 0.14          |
| (1,1892) | 1:30:A:LEU:HD23 | 1:68:A:GLU:H    | 14       | 0.14          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 19       | 0.14          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 19       | 0.14          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 19       | 0.14          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 19       | 0.14          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 19       | 0.14          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 19       | 0.14          |
| (1,1722) | 1:4:A:LEU:HD11  | 1:5:A:GLU:HA    | 2        | 0.14          |
| (1,1722) | 1:4:A:LEU:HD12  | 1:5:A:GLU:HA    | 2        | 0.14          |
| (1,1722) | 1:4:A:LEU:HD13  | 1:5:A:GLU:HA    | 2        | 0.14          |
| (1,1722) | 1:4:A:LEU:HD21  | 1:5:A:GLU:HA    | 2        | 0.14          |
| (1,1722) | 1:4:A:LEU:HD22  | 1:5:A:GLU:HA    | 2        | 0.14          |
| (1,1722) | 1:4:A:LEU:HD23  | 1:5:A:GLU:HA    | 2        | 0.14          |
| (1,1600) | 1:49:A:LEU:HD11 | 1:52:A:TYR:HD1  | 7        | 0.14          |
| (1,1600) | 1:49:A:LEU:HD11 | 1:52:A:TYR:HD2  | 7        | 0.14          |
| (1,1600) | 1:49:A:LEU:HD12 | 1:52:A:TYR:HD1  | 7        | 0.14          |
| (1,1600) | 1:49:A:LEU:HD12 | 1:52:A:TYR:HD2  | 7        | 0.14          |
| (1,1600) | 1:49:A:LEU:HD13 | 1:52:A:TYR:HD1  | 7        | 0.14          |
| (1,1600) | 1:49:A:LEU:HD13 | 1:52:A:TYR:HD2  | 7        | 0.14          |
| (1,1600) | 1:49:A:LEU:HD11 | 1:52:A:TYR:HD1  | 18       | 0.14          |
| (1,1600) | 1:49:A:LEU:HD11 | 1:52:A:TYR:HD2  | 18       | 0.14          |
| (1,1600) | 1:49:A:LEU:HD12 | 1:52:A:TYR:HD1  | 18       | 0.14          |
| (1,1600) | 1:49:A:LEU:HD12 | 1:52:A:TYR:HD2  | 18       | 0.14          |
| (1,1600) | 1:49:A:LEU:HD13 | 1:52:A:TYR:HD1  | 18       | 0.14          |
| (1,1600) | 1:49:A:LEU:HD13 | 1:52:A:TYR:HD2  | 18       | 0.14          |
| (1,1458) | 1:43:A:VAL:HG21 | 1:44:A:ASN:H    | 19       | 0.14          |
| (1,1458) | 1:43:A:VAL:HG22 | 1:44:A:ASN:H    | 19       | 0.14          |
| (1,1458) | 1:43:A:VAL:HG23 | 1:44:A:ASN:H    | 19       | 0.14          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB1  | 18       | 0.14          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB2  | 18       | 0.14          |
| (1,1190) | 1:3:A:HIS:HA    | 1:74:A:ALA:HB3  | 18       | 0.14          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD11 | 1        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD12 | 1        | 0.14          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD13 | 1        | 0.14          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD11 | 1        | 0.14          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD12 | 1        | 0.14          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD13 | 1        | 0.14          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD11 | 1        | 0.14          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD12 | 1        | 0.14          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD13 | 1        | 0.14          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD11 | 17       | 0.14          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD12 | 17       | 0.14          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD13 | 17       | 0.14          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD11 | 17       | 0.14          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD12 | 17       | 0.14          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD13 | 17       | 0.14          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD11 | 17       | 0.14          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD12 | 17       | 0.14          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD13 | 17       | 0.14          |
| (1,1091) | 1:50:A:GLU:HG2  | 1:57:A:VAL:HB   | 18       | 0.14          |
| (1,1091) | 1:50:A:GLU:HG3  | 1:57:A:VAL:HB   | 18       | 0.14          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 17       | 0.14          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 17       | 0.14          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 17       | 0.14          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 18       | 0.14          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 18       | 0.14          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 18       | 0.14          |
| (1,964)  | 2:84:A:PNS:H282 | 1:40:A:MET:HG2  | 6        | 0.14          |
| (1,964)  | 2:84:A:PNS:H282 | 1:40:A:MET:HG3  | 6        | 0.14          |
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 3        | 0.14          |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 3        | 0.14          |
| (1,933)  | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3  | 3        | 0.14          |
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 7        | 0.14          |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 7        | 0.14          |
| (1,933)  | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3  | 7        | 0.14          |
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 14       | 0.14          |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 14       | 0.14          |
| (1,933)  | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3  | 14       | 0.14          |
| (1,833)  | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 2        | 0.14          |
| (1,833)  | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 10       | 0.14          |
| (1,772)  | 1:10:A:ILE:HG21 | 1:13:A:ASP:HB2  | 11       | 0.14          |
| (1,772)  | 1:10:A:ILE:HG22 | 1:13:A:ASP:HB2  | 11       | 0.14          |
| (1,772)  | 1:10:A:ILE:HG23 | 1:13:A:ASP:HB2  | 11       | 0.14          |
| (1,676)  | 1:1:A:MET:HA    | 1:4:A:LEU:H     | 20       | 0.14          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,456) | 1:34:A:ILE:HB  | 1:36:A:GLU:H    | 3        | 0.14          |
| (1,456) | 1:34:A:ILE:HB  | 1:36:A:GLU:H    | 13       | 0.14          |
| (1,456) | 1:34:A:ILE:HB  | 1:36:A:GLU:H    | 17       | 0.14          |
| (1,400) | 1:5:A:GLU:HG2  | 1:6:A:ALA:H     | 3        | 0.14          |
| (1,400) | 1:5:A:GLU:HG3  | 1:6:A:ALA:H     | 3        | 0.14          |
| (1,299) | 1:13:A:ASP:HA  | 1:15:A:LEU:H    | 7        | 0.14          |
| (1,185) | 1:4:A:LEU:H    | 1:7:A:VAL:HB    | 1        | 0.14          |
| (1,185) | 1:4:A:LEU:H    | 1:7:A:VAL:HB    | 13       | 0.14          |
| (1,146) | 1:7:A:VAL:HG21 | 1:73:A:LEU:H    | 16       | 0.14          |
| (1,146) | 1:7:A:VAL:HG22 | 1:73:A:LEU:H    | 16       | 0.14          |
| (1,146) | 1:7:A:VAL:HG23 | 1:73:A:LEU:H    | 16       | 0.14          |
| (1,146) | 1:7:A:VAL:HG21 | 1:73:A:LEU:H    | 20       | 0.14          |
| (1,146) | 1:7:A:VAL:HG22 | 1:73:A:LEU:H    | 20       | 0.14          |
| (1,146) | 1:7:A:VAL:HG23 | 1:73:A:LEU:H    | 20       | 0.14          |
| (1,106) | 1:80:A:LYS:HD2 | 1:81:A:LEU:H    | 1        | 0.14          |
| (1,75)  | 1:16:A:ASN:H   | 1:16:A:ASN:HD21 | 19       | 0.14          |
| (1,44)  | 1:40:A:MET:HB3 | 1:43:A:VAL:H    | 1        | 0.14          |
| (1,41)  | 1:1:A:MET:HG2  | 1:4:A:LEU:H     | 8        | 0.14          |
| (1,41)  | 1:1:A:MET:HG2  | 1:4:A:LEU:H     | 11       | 0.14          |
| (1,7)   | 1:2:A:GLN:HE21 | 1:4:A:LEU:H     | 13       | 0.14          |
| (1,7)   | 1:2:A:GLN:HE21 | 1:4:A:LEU:H     | 16       | 0.14          |
| (2,93)  | 1:67:A:PHE:H   | 1:64:A:ALA:O    | 12       | 0.13          |
| (2,81)  | 1:13:A:ASP:H   | 1:9:A:ASN:O     | 16       | 0.13          |
| (2,74)  | 1:79:A:HIS:N   | 1:75:A:LEU:O    | 20       | 0.13          |
| (2,73)  | 1:79:A:HIS:H   | 1:75:A:LEU:O    | 14       | 0.13          |
| (2,73)  | 1:79:A:HIS:H   | 1:75:A:LEU:O    | 15       | 0.13          |
| (2,73)  | 1:79:A:HIS:H   | 1:75:A:LEU:O    | 18       | 0.13          |
| (2,67)  | 1:76:A:PHE:H   | 1:72:A:SER:O    | 14       | 0.13          |
| (2,61)  | 1:73:A:LEU:H   | 1:69:A:THR:O    | 1        | 0.13          |
| (2,61)  | 1:73:A:LEU:H   | 1:69:A:THR:O    | 5        | 0.13          |
| (2,61)  | 1:73:A:LEU:H   | 1:69:A:THR:O    | 13       | 0.13          |
| (2,61)  | 1:73:A:LEU:H   | 1:69:A:THR:O    | 18       | 0.13          |
| (2,59)  | 1:54:A:ASP:H   | 1:50:A:GLU:O    | 12       | 0.13          |
| (2,53)  | 1:51:A:GLU:H   | 1:47:A:THR:O    | 11       | 0.13          |
| (2,53)  | 1:51:A:GLU:H   | 1:47:A:THR:O    | 19       | 0.13          |
| (2,43)  | 1:46:A:ILE:H   | 1:42:A:VAL:O    | 16       | 0.13          |
| (2,33)  | 1:9:A:ASN:H    | 1:5:A:GLU:O     | 14       | 0.13          |
| (2,28)  | 1:76:A:PHE:O   | 1:80:A:LYS:N    | 3        | 0.13          |
| (2,28)  | 1:76:A:PHE:O   | 1:80:A:LYS:N    | 9        | 0.13          |
| (2,15)  | 1:46:A:ILE:O   | 1:49:A:LEU:N    | 8        | 0.13          |
| (2,1)   | 1:3:A:HIS:O    | 1:7:A:VAL:H     | 5        | 0.13          |
| (2,1)   | 1:3:A:HIS:O    | 1:7:A:VAL:H     | 15       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1)    | 1:3:A:HIS:O     | 1:7:A:VAL:H     | 19       | 0.13          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 11       | 0.13          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 11       | 0.13          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 11       | 0.13          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 11       | 0.13          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 11       | 0.13          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 11       | 0.13          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG21 | 8        | 0.13          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG22 | 8        | 0.13          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG23 | 8        | 0.13          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG21 | 8        | 0.13          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG22 | 8        | 0.13          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG23 | 8        | 0.13          |
| (1,1990) | 2:84:A:PNS:H311 | 1:40:A:MET:H    | 11       | 0.13          |
| (1,1990) | 2:84:A:PNS:H312 | 1:40:A:MET:H    | 11       | 0.13          |
| (1,1990) | 2:84:A:PNS:H313 | 1:40:A:MET:H    | 11       | 0.13          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 11       | 0.13          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 11       | 0.13          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 11       | 0.13          |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 11       | 0.13          |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 11       | 0.13          |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 11       | 0.13          |
| (1,1977) | 2:84:A:PNS:H311 | 1:40:A:MET:H    | 11       | 0.13          |
| (1,1977) | 2:84:A:PNS:H312 | 1:40:A:MET:H    | 11       | 0.13          |
| (1,1977) | 2:84:A:PNS:H313 | 1:40:A:MET:H    | 11       | 0.13          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD11 | 2        | 0.13          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD12 | 2        | 0.13          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD13 | 2        | 0.13          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD21 | 2        | 0.13          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD22 | 2        | 0.13          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD23 | 2        | 0.13          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD11 | 2        | 0.13          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD12 | 2        | 0.13          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD13 | 2        | 0.13          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD21 | 2        | 0.13          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD22 | 2        | 0.13          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD23 | 2        | 0.13          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD11 | 7        | 0.13          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD12 | 7        | 0.13          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD13 | 7        | 0.13          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD21 | 7        | 0.13          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD22 | 7        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD23 | 7        | 0.13          |
| (1,1722) | 1:4:A:LEU:HD11  | 1:5:A:GLU:HA    | 7        | 0.13          |
| (1,1722) | 1:4:A:LEU:HD12  | 1:5:A:GLU:HA    | 7        | 0.13          |
| (1,1722) | 1:4:A:LEU:HD13  | 1:5:A:GLU:HA    | 7        | 0.13          |
| (1,1722) | 1:4:A:LEU:HD21  | 1:5:A:GLU:HA    | 7        | 0.13          |
| (1,1722) | 1:4:A:LEU:HD22  | 1:5:A:GLU:HA    | 7        | 0.13          |
| (1,1722) | 1:4:A:LEU:HD23  | 1:5:A:GLU:HA    | 7        | 0.13          |
| (1,1666) | 1:55:A:PHE:HZ   | 1:57:A:VAL:HB   | 6        | 0.13          |
| (1,1666) | 1:55:A:PHE:HZ   | 1:57:A:VAL:HB   | 8        | 0.13          |
| (1,1388) | 1:24:A:LEU:HD11 | 1:25:A:THR:HA   | 14       | 0.13          |
| (1,1388) | 1:24:A:LEU:HD12 | 1:25:A:THR:HA   | 14       | 0.13          |
| (1,1388) | 1:24:A:LEU:HD13 | 1:25:A:THR:HA   | 14       | 0.13          |
| (1,1139) | 1:66:A:THR:HG21 | 1:76:A:PHE:HB2  | 9        | 0.13          |
| (1,1139) | 1:66:A:THR:HG22 | 1:76:A:PHE:HB2  | 9        | 0.13          |
| (1,1139) | 1:66:A:THR:HG23 | 1:76:A:PHE:HB2  | 9        | 0.13          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD11 | 19       | 0.13          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD12 | 19       | 0.13          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD13 | 19       | 0.13          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD11 | 19       | 0.13          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD12 | 19       | 0.13          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD13 | 19       | 0.13          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD11 | 19       | 0.13          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD12 | 19       | 0.13          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD13 | 19       | 0.13          |
| (1,1091) | 1:50:A:GLU:HG2  | 1:57:A:VAL:HB   | 2        | 0.13          |
| (1,1091) | 1:50:A:GLU:HG3  | 1:57:A:VAL:HB   | 2        | 0.13          |
| (1,1021) | 1:45:A:VAL:HB   | 1:46:A:ILE:HG13 | 3        | 0.13          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 16       | 0.13          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 16       | 0.13          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 16       | 0.13          |
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 16       | 0.13          |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 16       | 0.13          |
| (1,933)  | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3  | 16       | 0.13          |
| (1,916)  | 1:31:A:LEU:HG   | 1:67:A:PHE:H    | 6        | 0.13          |
| (1,864)  | 1:8:A:ARG:HD2   | 1:24:A:LEU:HD21 | 9        | 0.13          |
| (1,864)  | 1:8:A:ARG:HD2   | 1:24:A:LEU:HD22 | 9        | 0.13          |
| (1,864)  | 1:8:A:ARG:HD2   | 1:24:A:LEU:HD23 | 9        | 0.13          |
| (1,833)  | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 17       | 0.13          |
| (1,676)  | 1:1:A:MET:HA    | 1:4:A:LEU:H     | 19       | 0.13          |
| (1,649)  | 1:6:A:ALA:HB1   | 1:9:A:ASN:HD22  | 1        | 0.13          |
| (1,649)  | 1:6:A:ALA:HB2   | 1:9:A:ASN:HD22  | 1        | 0.13          |
| (1,649)  | 1:6:A:ALA:HB3   | 1:9:A:ASN:HD22  | 1        | 0.13          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,456) | 1:34:A:ILE:HB   | 1:36:A:GLU:H   | 2        | 0.13          |
| (1,456) | 1:34:A:ILE:HB   | 1:36:A:GLU:H   | 4        | 0.13          |
| (1,456) | 1:34:A:ILE:HB   | 1:36:A:GLU:H   | 9        | 0.13          |
| (1,456) | 1:34:A:ILE:HB   | 1:36:A:GLU:H   | 18       | 0.13          |
| (1,456) | 1:34:A:ILE:HB   | 1:36:A:GLU:H   | 19       | 0.13          |
| (1,185) | 1:4:A:LEU:H     | 1:7:A:VAL:HB   | 2        | 0.13          |
| (1,185) | 1:4:A:LEU:H     | 1:7:A:VAL:HB   | 5        | 0.13          |
| (1,185) | 1:4:A:LEU:H     | 1:7:A:VAL:HB   | 14       | 0.13          |
| (1,146) | 1:7:A:VAL:HG21  | 1:73:A:LEU:H   | 6        | 0.13          |
| (1,146) | 1:7:A:VAL:HG22  | 1:73:A:LEU:H   | 6        | 0.13          |
| (1,146) | 1:7:A:VAL:HG23  | 1:73:A:LEU:H   | 6        | 0.13          |
| (1,146) | 1:7:A:VAL:HG21  | 1:73:A:LEU:H   | 13       | 0.13          |
| (1,146) | 1:7:A:VAL:HG22  | 1:73:A:LEU:H   | 13       | 0.13          |
| (1,146) | 1:7:A:VAL:HG23  | 1:73:A:LEU:H   | 13       | 0.13          |
| (1,45)  | 2:84:A:PNS:H281 | 1:40:A:MET:H   | 1        | 0.13          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG21 | 6        | 0.13          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG22 | 6        | 0.13          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG23 | 6        | 0.13          |
| (1,13)  | 1:19:A:GLU:HG2  | 1:22:A:HIS:H   | 19       | 0.13          |
| (1,13)  | 1:19:A:GLU:HG3  | 1:22:A:HIS:H   | 19       | 0.13          |
| (1,7)   | 1:2:A:GLN:HE21  | 1:4:A:LEU:H    | 8        | 0.13          |
| (2,93)  | 1:67:A:PHE:H    | 1:64:A:ALA:O   | 17       | 0.12          |
| (2,91)  | 1:66:A:THR:H    | 1:63:A:SER:O   | 13       | 0.12          |
| (2,81)  | 1:13:A:ASP:H    | 1:9:A:ASN:O    | 5        | 0.12          |
| (2,81)  | 1:13:A:ASP:H    | 1:9:A:ASN:O    | 13       | 0.12          |
| (2,81)  | 1:13:A:ASP:H    | 1:9:A:ASN:O    | 20       | 0.12          |
| (2,75)  | 1:80:A:LYS:H    | 1:76:A:PHE:O   | 2        | 0.12          |
| (2,75)  | 1:80:A:LYS:H    | 1:76:A:PHE:O   | 7        | 0.12          |
| (2,75)  | 1:80:A:LYS:H    | 1:76:A:PHE:O   | 8        | 0.12          |
| (2,75)  | 1:80:A:LYS:H    | 1:76:A:PHE:O   | 13       | 0.12          |
| (2,74)  | 1:79:A:HIS:N    | 1:75:A:LEU:O   | 4        | 0.12          |
| (2,62)  | 1:73:A:LEU:N    | 1:69:A:THR:O   | 20       | 0.12          |
| (2,61)  | 1:73:A:LEU:H    | 1:69:A:THR:O   | 4        | 0.12          |
| (2,61)  | 1:73:A:LEU:H    | 1:69:A:THR:O   | 8        | 0.12          |
| (2,61)  | 1:73:A:LEU:H    | 1:69:A:THR:O   | 17       | 0.12          |
| (2,57)  | 1:53:A:PHE:H    | 1:49:A:LEU:O   | 9        | 0.12          |
| (2,57)  | 1:53:A:PHE:H    | 1:49:A:LEU:O   | 15       | 0.12          |
| (2,53)  | 1:51:A:GLU:H    | 1:47:A:THR:O   | 14       | 0.12          |
| (2,43)  | 1:46:A:ILE:H    | 1:42:A:VAL:O   | 13       | 0.12          |
| (2,35)  | 1:10:A:ILE:H    | 1:6:A:ALA:O    | 7        | 0.12          |
| (2,33)  | 1:9:A:ASN:H     | 1:5:A:GLU:O    | 12       | 0.12          |
| (2,33)  | 1:9:A:ASN:H     | 1:5:A:GLU:O    | 15       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,28)   | 1:76:A:PHE:O    | 1:80:A:LYS:N    | 20       | 0.12          |
| (2,2)    | 1:3:A:HIS:O     | 1:7:A:VAL:N     | 3        | 0.12          |
| (2,2)    | 1:3:A:HIS:O     | 1:7:A:VAL:N     | 6        | 0.12          |
| (2,1)    | 1:3:A:HIS:O     | 1:7:A:VAL:H     | 4        | 0.12          |
| (2,1)    | 1:3:A:HIS:O     | 1:7:A:VAL:H     | 8        | 0.12          |
| (2,1)    | 1:3:A:HIS:O     | 1:7:A:VAL:H     | 10       | 0.12          |
| (2,1)    | 1:3:A:HIS:O     | 1:7:A:VAL:H     | 13       | 0.12          |
| (2,1)    | 1:3:A:HIS:O     | 1:7:A:VAL:H     | 17       | 0.12          |
| (2,1)    | 1:3:A:HIS:O     | 1:7:A:VAL:H     | 20       | 0.12          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 9        | 0.12          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 9        | 0.12          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 9        | 0.12          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 9        | 0.12          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 9        | 0.12          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 9        | 0.12          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 13       | 0.12          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 13       | 0.12          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 13       | 0.12          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 13       | 0.12          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 13       | 0.12          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 13       | 0.12          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG21 | 16       | 0.12          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG22 | 16       | 0.12          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG23 | 16       | 0.12          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG21 | 16       | 0.12          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG22 | 16       | 0.12          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG23 | 16       | 0.12          |
| (1,1992) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG21 | 10       | 0.12          |
| (1,1992) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG22 | 10       | 0.12          |
| (1,1992) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG23 | 10       | 0.12          |
| (1,1992) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG21 | 10       | 0.12          |
| (1,1992) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG22 | 10       | 0.12          |
| (1,1992) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG23 | 10       | 0.12          |
| (1,1992) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG21 | 10       | 0.12          |
| (1,1992) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG22 | 10       | 0.12          |
| (1,1992) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG23 | 10       | 0.12          |
| (1,1990) | 2:84:A:PNS:H311 | 1:40:A:MET:H    | 15       | 0.12          |
| (1,1990) | 2:84:A:PNS:H312 | 1:40:A:MET:H    | 15       | 0.12          |
| (1,1990) | 2:84:A:PNS:H313 | 1:40:A:MET:H    | 15       | 0.12          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 9        | 0.12          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 9        | 0.12          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 9        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 9        | 0.12          |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 9        | 0.12          |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 9        | 0.12          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 13       | 0.12          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 13       | 0.12          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 13       | 0.12          |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 13       | 0.12          |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 13       | 0.12          |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 13       | 0.12          |
| (1,1979) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG21 | 10       | 0.12          |
| (1,1979) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG22 | 10       | 0.12          |
| (1,1979) | 2:84:A:PNS:H301 | 1:42:A:VAL:HG23 | 10       | 0.12          |
| (1,1979) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG21 | 10       | 0.12          |
| (1,1979) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG22 | 10       | 0.12          |
| (1,1979) | 2:84:A:PNS:H302 | 1:42:A:VAL:HG23 | 10       | 0.12          |
| (1,1979) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG21 | 10       | 0.12          |
| (1,1979) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG22 | 10       | 0.12          |
| (1,1979) | 2:84:A:PNS:H303 | 1:42:A:VAL:HG23 | 10       | 0.12          |
| (1,1977) | 2:84:A:PNS:H311 | 1:40:A:MET:H    | 15       | 0.12          |
| (1,1977) | 2:84:A:PNS:H312 | 1:40:A:MET:H    | 15       | 0.12          |
| (1,1977) | 2:84:A:PNS:H313 | 1:40:A:MET:H    | 15       | 0.12          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD11 | 18       | 0.12          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD12 | 18       | 0.12          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD13 | 18       | 0.12          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD21 | 18       | 0.12          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD22 | 18       | 0.12          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD23 | 18       | 0.12          |
| (1,1889) | 1:30:A:LEU:HD11 | 1:67:A:PHE:HB2  | 14       | 0.12          |
| (1,1889) | 1:30:A:LEU:HD12 | 1:67:A:PHE:HB2  | 14       | 0.12          |
| (1,1889) | 1:30:A:LEU:HD13 | 1:67:A:PHE:HB2  | 14       | 0.12          |
| (1,1889) | 1:30:A:LEU:HD21 | 1:67:A:PHE:HB2  | 14       | 0.12          |
| (1,1889) | 1:30:A:LEU:HD22 | 1:67:A:PHE:HB2  | 14       | 0.12          |
| (1,1889) | 1:30:A:LEU:HD23 | 1:67:A:PHE:HB2  | 14       | 0.12          |
| (1,1767) | 1:11:A:LEU:HD11 | 1:67:A:PHE:HD1  | 7        | 0.12          |
| (1,1767) | 1:11:A:LEU:HD11 | 1:67:A:PHE:HD2  | 7        | 0.12          |
| (1,1767) | 1:11:A:LEU:HD12 | 1:67:A:PHE:HD1  | 7        | 0.12          |
| (1,1767) | 1:11:A:LEU:HD12 | 1:67:A:PHE:HD2  | 7        | 0.12          |
| (1,1767) | 1:11:A:LEU:HD13 | 1:67:A:PHE:HD1  | 7        | 0.12          |
| (1,1767) | 1:11:A:LEU:HD13 | 1:67:A:PHE:HD2  | 7        | 0.12          |
| (1,1767) | 1:11:A:LEU:HD21 | 1:67:A:PHE:HD1  | 7        | 0.12          |
| (1,1767) | 1:11:A:LEU:HD21 | 1:67:A:PHE:HD2  | 7        | 0.12          |
| (1,1767) | 1:11:A:LEU:HD22 | 1:67:A:PHE:HD1  | 7        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1767) | 1:11:A:LEU:HD22 | 1:67:A:PHE:HD2  | 7        | 0.12          |
| (1,1767) | 1:11:A:LEU:HD23 | 1:67:A:PHE:HD1  | 7        | 0.12          |
| (1,1767) | 1:11:A:LEU:HD23 | 1:67:A:PHE:HD2  | 7        | 0.12          |
| (1,1722) | 1:4:A:LEU:HD11  | 1:5:A:GLU:HA    | 15       | 0.12          |
| (1,1722) | 1:4:A:LEU:HD12  | 1:5:A:GLU:HA    | 15       | 0.12          |
| (1,1722) | 1:4:A:LEU:HD13  | 1:5:A:GLU:HA    | 15       | 0.12          |
| (1,1722) | 1:4:A:LEU:HD21  | 1:5:A:GLU:HA    | 15       | 0.12          |
| (1,1722) | 1:4:A:LEU:HD22  | 1:5:A:GLU:HA    | 15       | 0.12          |
| (1,1722) | 1:4:A:LEU:HD23  | 1:5:A:GLU:HA    | 15       | 0.12          |
| (1,1388) | 1:24:A:LEU:HD11 | 1:25:A:THR:HA   | 20       | 0.12          |
| (1,1388) | 1:24:A:LEU:HD12 | 1:25:A:THR:HA   | 20       | 0.12          |
| (1,1388) | 1:24:A:LEU:HD13 | 1:25:A:THR:HA   | 20       | 0.12          |
| (1,1237) | 1:79:A:HIS:HB2  | 1:82:A:SER:H    | 13       | 0.12          |
| (1,1237) | 1:79:A:HIS:HB3  | 1:82:A:SER:H    | 13       | 0.12          |
| (1,1208) | 1:57:A:VAL:HG21 | 1:77:A:VAL:HA   | 11       | 0.12          |
| (1,1208) | 1:57:A:VAL:HG22 | 1:77:A:VAL:HA   | 11       | 0.12          |
| (1,1208) | 1:57:A:VAL:HG23 | 1:77:A:VAL:HA   | 11       | 0.12          |
| (1,1159) | 1:30:A:LEU:HD21 | 1:69:A:THR:HB   | 12       | 0.12          |
| (1,1159) | 1:30:A:LEU:HD22 | 1:69:A:THR:HB   | 12       | 0.12          |
| (1,1159) | 1:30:A:LEU:HD23 | 1:69:A:THR:HB   | 12       | 0.12          |
| (1,1139) | 1:66:A:THR:HG21 | 1:76:A:PHE:HB2  | 19       | 0.12          |
| (1,1139) | 1:66:A:THR:HG22 | 1:76:A:PHE:HB2  | 19       | 0.12          |
| (1,1139) | 1:66:A:THR:HG23 | 1:76:A:PHE:HB2  | 19       | 0.12          |
| (1,1132) | 1:66:A:THR:HA   | 1:67:A:PHE:HD1  | 7        | 0.12          |
| (1,1132) | 1:66:A:THR:HA   | 1:67:A:PHE:HD2  | 7        | 0.12          |
| (1,1091) | 1:50:A:GLU:HG2  | 1:57:A:VAL:HB   | 20       | 0.12          |
| (1,1091) | 1:50:A:GLU:HG3  | 1:57:A:VAL:HB   | 20       | 0.12          |
| (1,1021) | 1:45:A:VAL:HB   | 1:46:A:ILE:HG13 | 20       | 0.12          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG21 | 9        | 0.12          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG22 | 9        | 0.12          |
| (1,1000) | 1:44:A:ASN:HA   | 1:45:A:VAL:HG23 | 9        | 0.12          |
| (1,995)  | 1:43:A:VAL:HG21 | 1:44:A:ASN:HB2  | 19       | 0.12          |
| (1,995)  | 1:43:A:VAL:HG22 | 1:44:A:ASN:HB2  | 19       | 0.12          |
| (1,995)  | 1:43:A:VAL:HG23 | 1:44:A:ASN:HB2  | 19       | 0.12          |
| (1,971)  | 1:41:A:ALA:HA   | 1:44:A:ASN:HD22 | 6        | 0.12          |
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 8        | 0.12          |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 8        | 0.12          |
| (1,933)  | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3  | 8        | 0.12          |
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 12       | 0.12          |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 12       | 0.12          |
| (1,933)  | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3  | 12       | 0.12          |
| (1,870)  | 1:23:A:THR:H    | 1:24:A:LEU:HD11 | 14       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,870) | 1:23:A:THR:H    | 1:24:A:LEU:HD12 | 14       | 0.12          |
| (1,870) | 1:23:A:THR:H    | 1:24:A:LEU:HD13 | 14       | 0.12          |
| (1,833) | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 11       | 0.12          |
| (1,833) | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 12       | 0.12          |
| (1,811) | 1:19:A:GLU:HA   | 1:21:A:LYS:HE2  | 13       | 0.12          |
| (1,811) | 1:19:A:GLU:HA   | 1:21:A:LYS:HE3  | 13       | 0.12          |
| (1,772) | 1:10:A:ILE:HG21 | 1:13:A:ASP:HB2  | 9        | 0.12          |
| (1,772) | 1:10:A:ILE:HG22 | 1:13:A:ASP:HB2  | 9        | 0.12          |
| (1,772) | 1:10:A:ILE:HG23 | 1:13:A:ASP:HB2  | 9        | 0.12          |
| (1,772) | 1:10:A:ILE:HG21 | 1:13:A:ASP:HB2  | 20       | 0.12          |
| (1,772) | 1:10:A:ILE:HG22 | 1:13:A:ASP:HB2  | 20       | 0.12          |
| (1,772) | 1:10:A:ILE:HG23 | 1:13:A:ASP:HB2  | 20       | 0.12          |
| (1,741) | 1:8:A:ARG:HG3   | 1:9:A:ASN:HA    | 1        | 0.12          |
| (1,741) | 1:8:A:ARG:HG3   | 1:9:A:ASN:HA    | 6        | 0.12          |
| (1,675) | 1:64:A:ALA:HA   | 1:65:A:GLN:HE21 | 6        | 0.12          |
| (1,400) | 1:5:A:GLU:HG2   | 1:6:A:ALA:H     | 7        | 0.12          |
| (1,400) | 1:5:A:GLU:HG3   | 1:6:A:ALA:H     | 7        | 0.12          |
| (1,366) | 1:11:A:LEU:HA   | 1:14:A:VAL:H    | 8        | 0.12          |
| (1,366) | 1:11:A:LEU:HA   | 1:14:A:VAL:H    | 15       | 0.12          |
| (1,366) | 1:11:A:LEU:HA   | 1:14:A:VAL:H    | 16       | 0.12          |
| (1,299) | 1:13:A:ASP:HA   | 1:15:A:LEU:H    | 15       | 0.12          |
| (1,256) | 1:1:A:MET:HG3   | 1:4:A:LEU:H     | 7        | 0.12          |
| (1,256) | 1:1:A:MET:HG3   | 1:4:A:LEU:H     | 14       | 0.12          |
| (1,225) | 1:9:A:ASN:H     | 1:21:A:LYS:HE2  | 2        | 0.12          |
| (1,225) | 1:9:A:ASN:H     | 1:21:A:LYS:HE3  | 2        | 0.12          |
| (1,185) | 1:4:A:LEU:H     | 1:7:A:VAL:HB    | 8        | 0.12          |
| (1,185) | 1:4:A:LEU:H     | 1:7:A:VAL:HB    | 10       | 0.12          |
| (1,181) | 1:2:A:GLN:HA    | 1:5:A:GLU:H     | 2        | 0.12          |
| (1,164) | 1:30:A:LEU:H    | 1:69:A:THR:HB   | 17       | 0.12          |
| (1,106) | 1:80:A:LYS:HD2  | 1:81:A:LEU:H    | 10       | 0.12          |
| (1,106) | 1:80:A:LYS:HD2  | 1:81:A:LEU:H    | 12       | 0.12          |
| (1,106) | 1:80:A:LYS:HD2  | 1:81:A:LEU:H    | 17       | 0.12          |
| (1,44)  | 1:40:A:MET:HB3  | 1:43:A:VAL:H    | 5        | 0.12          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG21  | 3        | 0.12          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG22  | 3        | 0.12          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG23  | 3        | 0.12          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG21  | 14       | 0.12          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG22  | 14       | 0.12          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG23  | 14       | 0.12          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG21  | 15       | 0.12          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG22  | 15       | 0.12          |
| (1,25)  | 1:3:A:HIS:H     | 1:7:A:VAL:HG23  | 15       | 0.12          |

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| Key    | Atom-1         | Atom-2       | Model ID | Violation (Å) |
|--------|----------------|--------------|----------|---------------|
| (1,22) | 1:55:A:PHE:HD1 | 1:58:A:ASP:H | 18       | 0.12          |
| (1,22) | 1:55:A:PHE:HD2 | 1:58:A:ASP:H | 18       | 0.12          |
| (1,13) | 1:19:A:GLU:HG2 | 1:22:A:HIS:H | 11       | 0.12          |
| (1,13) | 1:19:A:GLU:HG3 | 1:22:A:HIS:H | 11       | 0.12          |
| (1,12) | 1:2:A:GLN:H    | 1:5:A:GLU:H  | 8        | 0.12          |
| (2,93) | 1:67:A:PHE:H   | 1:64:A:ALA:O | 3        | 0.11          |
| (2,93) | 1:67:A:PHE:H   | 1:64:A:ALA:O | 8        | 0.11          |
| (2,81) | 1:13:A:ASP:H   | 1:9:A:ASN:O  | 3        | 0.11          |
| (2,81) | 1:13:A:ASP:H   | 1:9:A:ASN:O  | 8        | 0.11          |
| (2,75) | 1:80:A:LYS:H   | 1:76:A:PHE:O | 10       | 0.11          |
| (2,74) | 1:79:A:HIS:N   | 1:75:A:LEU:O | 11       | 0.11          |
| (2,73) | 1:79:A:HIS:H   | 1:75:A:LEU:O | 3        | 0.11          |
| (2,73) | 1:79:A:HIS:H   | 1:75:A:LEU:O | 7        | 0.11          |
| (2,62) | 1:73:A:LEU:N   | 1:69:A:THR:O | 9        | 0.11          |
| (2,62) | 1:73:A:LEU:N   | 1:69:A:THR:O | 19       | 0.11          |
| (2,61) | 1:73:A:LEU:H   | 1:69:A:THR:O | 14       | 0.11          |
| (2,55) | 1:52:A:TYR:H   | 1:48:A:ALA:O | 18       | 0.11          |
| (2,53) | 1:51:A:GLU:H   | 1:47:A:THR:O | 6        | 0.11          |
| (2,51) | 1:50:A:GLU:H   | 1:46:A:ILE:O | 9        | 0.11          |
| (2,51) | 1:50:A:GLU:H   | 1:46:A:ILE:O | 15       | 0.11          |
| (2,45) | 1:47:A:THR:H   | 1:43:A:VAL:O | 8        | 0.11          |
| (2,44) | 1:46:A:ILE:N   | 1:42:A:VAL:O | 10       | 0.11          |
| (2,43) | 1:46:A:ILE:H   | 1:42:A:VAL:O | 6        | 0.11          |
| (2,43) | 1:46:A:ILE:H   | 1:42:A:VAL:O | 11       | 0.11          |
| (2,43) | 1:46:A:ILE:H   | 1:42:A:VAL:O | 14       | 0.11          |
| (2,43) | 1:46:A:ILE:H   | 1:42:A:VAL:O | 17       | 0.11          |
| (2,43) | 1:46:A:ILE:H   | 1:42:A:VAL:O | 18       | 0.11          |
| (2,43) | 1:46:A:ILE:H   | 1:42:A:VAL:O | 20       | 0.11          |
| (2,35) | 1:10:A:ILE:H   | 1:6:A:ALA:O  | 8        | 0.11          |
| (2,35) | 1:10:A:ILE:H   | 1:6:A:ALA:O  | 10       | 0.11          |
| (2,35) | 1:10:A:ILE:H   | 1:6:A:ALA:O  | 16       | 0.11          |
| (2,33) | 1:9:A:ASN:H    | 1:5:A:GLU:O  | 5        | 0.11          |
| (2,33) | 1:9:A:ASN:H    | 1:5:A:GLU:O  | 9        | 0.11          |
| (2,28) | 1:76:A:PHE:O   | 1:80:A:LYS:N | 1        | 0.11          |
| (2,28) | 1:76:A:PHE:O   | 1:80:A:LYS:N | 14       | 0.11          |
| (2,21) | 1:50:A:GLU:O   | 1:54:A:ASP:N | 12       | 0.11          |
| (2,21) | 1:50:A:GLU:O   | 1:54:A:ASP:N | 14       | 0.11          |
| (2,12) | 1:41:A:ALA:O   | 1:45:A:VAL:H | 7        | 0.11          |
| (2,12) | 1:41:A:ALA:O   | 1:45:A:VAL:H | 10       | 0.11          |
| (2,2)  | 1:3:A:HIS:O    | 1:7:A:VAL:N  | 2        | 0.11          |
| (2,2)  | 1:3:A:HIS:O    | 1:7:A:VAL:N  | 4        | 0.11          |
| (2,2)  | 1:3:A:HIS:O    | 1:7:A:VAL:N  | 7        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,2)    | 1:3:A:HIS:O     | 1:7:A:VAL:N     | 12       | 0.11          |
| (2,2)    | 1:3:A:HIS:O     | 1:7:A:VAL:N     | 14       | 0.11          |
| (2,2)    | 1:3:A:HIS:O     | 1:7:A:VAL:N     | 19       | 0.11          |
| (2,1)    | 1:3:A:HIS:O     | 1:7:A:VAL:H     | 7        | 0.11          |
| (2,1)    | 1:3:A:HIS:O     | 1:7:A:VAL:H     | 16       | 0.11          |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG21 | 1        | 0.11          |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG22 | 1        | 0.11          |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG23 | 1        | 0.11          |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG21 | 1        | 0.11          |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG22 | 1        | 0.11          |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG23 | 1        | 0.11          |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG21 | 8        | 0.11          |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG22 | 8        | 0.11          |
| (1,2009) | 2:84:A:PNS:H431 | 1:43:A:VAL:HG23 | 8        | 0.11          |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG21 | 8        | 0.11          |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG22 | 8        | 0.11          |
| (1,2009) | 2:84:A:PNS:H432 | 1:43:A:VAL:HG23 | 8        | 0.11          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 5        | 0.11          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 5        | 0.11          |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 5        | 0.11          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 5        | 0.11          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 5        | 0.11          |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 5        | 0.11          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG21 | 15       | 0.11          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG22 | 15       | 0.11          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG23 | 15       | 0.11          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG21 | 15       | 0.11          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG22 | 15       | 0.11          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG23 | 15       | 0.11          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG21 | 20       | 0.11          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG22 | 20       | 0.11          |
| (1,2003) | 2:84:A:PNS:H421 | 1:43:A:VAL:HG23 | 20       | 0.11          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG21 | 20       | 0.11          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG22 | 20       | 0.11          |
| (1,2003) | 2:84:A:PNS:H422 | 1:43:A:VAL:HG23 | 20       | 0.11          |
| (1,1994) | 2:84:A:PNS:H371 | 1:46:A:ILE:HD11 | 4        | 0.11          |
| (1,1994) | 2:84:A:PNS:H371 | 1:46:A:ILE:HD12 | 4        | 0.11          |
| (1,1994) | 2:84:A:PNS:H371 | 1:46:A:ILE:HD13 | 4        | 0.11          |
| (1,1994) | 2:84:A:PNS:H372 | 1:46:A:ILE:HD11 | 4        | 0.11          |
| (1,1994) | 2:84:A:PNS:H372 | 1:46:A:ILE:HD12 | 4        | 0.11          |
| (1,1994) | 2:84:A:PNS:H372 | 1:46:A:ILE:HD13 | 4        | 0.11          |
| (1,1990) | 2:84:A:PNS:H311 | 1:40:A:MET:H    | 9        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1990) | 2:84:A:PNS:H312 | 1:40:A:MET:H    | 9        | 0.11          |
| (1,1990) | 2:84:A:PNS:H313 | 1:40:A:MET:H    | 9        | 0.11          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 5        | 0.11          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 5        | 0.11          |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 5        | 0.11          |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 5        | 0.11          |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 5        | 0.11          |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 5        | 0.11          |
| (1,1977) | 2:84:A:PNS:H311 | 1:40:A:MET:H    | 9        | 0.11          |
| (1,1977) | 2:84:A:PNS:H312 | 1:40:A:MET:H    | 9        | 0.11          |
| (1,1977) | 2:84:A:PNS:H313 | 1:40:A:MET:H    | 9        | 0.11          |
| (1,1957) | 2:84:A:PNS:H371 | 1:43:A:VAL:HG11 | 11       | 0.11          |
| (1,1957) | 2:84:A:PNS:H371 | 1:43:A:VAL:HG12 | 11       | 0.11          |
| (1,1957) | 2:84:A:PNS:H371 | 1:43:A:VAL:HG13 | 11       | 0.11          |
| (1,1957) | 2:84:A:PNS:H372 | 1:43:A:VAL:HG11 | 11       | 0.11          |
| (1,1957) | 2:84:A:PNS:H372 | 1:43:A:VAL:HG12 | 11       | 0.11          |
| (1,1957) | 2:84:A:PNS:H372 | 1:43:A:VAL:HG13 | 11       | 0.11          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD11 | 7        | 0.11          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD12 | 7        | 0.11          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD13 | 7        | 0.11          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD21 | 7        | 0.11          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD22 | 7        | 0.11          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD23 | 7        | 0.11          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD11 | 7        | 0.11          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD12 | 7        | 0.11          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD13 | 7        | 0.11          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD21 | 7        | 0.11          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD22 | 7        | 0.11          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD23 | 7        | 0.11          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD11 | 19       | 0.11          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD12 | 19       | 0.11          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD13 | 19       | 0.11          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD21 | 19       | 0.11          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD22 | 19       | 0.11          |
| (1,1924) | 1:32:A:GLY:HA2  | 1:37:A:LEU:HD23 | 19       | 0.11          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD11 | 19       | 0.11          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD12 | 19       | 0.11          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD13 | 19       | 0.11          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD21 | 19       | 0.11          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD22 | 19       | 0.11          |
| (1,1924) | 1:32:A:GLY:HA3  | 1:37:A:LEU:HD23 | 19       | 0.11          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD11 | 11       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD12 | 11       | 0.11          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD13 | 11       | 0.11          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD21 | 11       | 0.11          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD22 | 11       | 0.11          |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD23 | 11       | 0.11          |
| (1,1889) | 1:30:A:LEU:HD11 | 1:67:A:PHE:HB2  | 6        | 0.11          |
| (1,1889) | 1:30:A:LEU:HD12 | 1:67:A:PHE:HB2  | 6        | 0.11          |
| (1,1889) | 1:30:A:LEU:HD13 | 1:67:A:PHE:HB2  | 6        | 0.11          |
| (1,1889) | 1:30:A:LEU:HD21 | 1:67:A:PHE:HB2  | 6        | 0.11          |
| (1,1889) | 1:30:A:LEU:HD22 | 1:67:A:PHE:HB2  | 6        | 0.11          |
| (1,1889) | 1:30:A:LEU:HD23 | 1:67:A:PHE:HB2  | 6        | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 7        | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 7        | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 7        | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 7        | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 7        | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 7        | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 11       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 11       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 11       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 11       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 11       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 11       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 15       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 15       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 15       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 15       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 15       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 15       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 17       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 17       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 17       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 17       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 17       | 0.11          |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 17       | 0.11          |
| (1,1823) | 1:15:A:LEU:HD11 | 1:44:A:ASN:HD21 | 9        | 0.11          |
| (1,1823) | 1:15:A:LEU:HD12 | 1:44:A:ASN:HD21 | 9        | 0.11          |
| (1,1823) | 1:15:A:LEU:HD13 | 1:44:A:ASN:HD21 | 9        | 0.11          |
| (1,1823) | 1:15:A:LEU:HD21 | 1:44:A:ASN:HD21 | 9        | 0.11          |
| (1,1823) | 1:15:A:LEU:HD22 | 1:44:A:ASN:HD21 | 9        | 0.11          |
| (1,1823) | 1:15:A:LEU:HD23 | 1:44:A:ASN:HD21 | 9        | 0.11          |
| (1,1722) | 1:4:A:LEU:HD11  | 1:5:A:GLU:HA    | 3        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1722) | 1:4:A:LEU:HD12  | 1:5:A:GLU:HA    | 3        | 0.11          |
| (1,1722) | 1:4:A:LEU:HD13  | 1:5:A:GLU:HA    | 3        | 0.11          |
| (1,1722) | 1:4:A:LEU:HD21  | 1:5:A:GLU:HA    | 3        | 0.11          |
| (1,1722) | 1:4:A:LEU:HD22  | 1:5:A:GLU:HA    | 3        | 0.11          |
| (1,1722) | 1:4:A:LEU:HD23  | 1:5:A:GLU:HA    | 3        | 0.11          |
| (1,1722) | 1:4:A:LEU:HD11  | 1:5:A:GLU:HA    | 13       | 0.11          |
| (1,1722) | 1:4:A:LEU:HD12  | 1:5:A:GLU:HA    | 13       | 0.11          |
| (1,1722) | 1:4:A:LEU:HD13  | 1:5:A:GLU:HA    | 13       | 0.11          |
| (1,1722) | 1:4:A:LEU:HD21  | 1:5:A:GLU:HA    | 13       | 0.11          |
| (1,1722) | 1:4:A:LEU:HD22  | 1:5:A:GLU:HA    | 13       | 0.11          |
| (1,1722) | 1:4:A:LEU:HD23  | 1:5:A:GLU:HA    | 13       | 0.11          |
| (1,1722) | 1:4:A:LEU:HD11  | 1:5:A:GLU:HA    | 14       | 0.11          |
| (1,1722) | 1:4:A:LEU:HD12  | 1:5:A:GLU:HA    | 14       | 0.11          |
| (1,1722) | 1:4:A:LEU:HD13  | 1:5:A:GLU:HA    | 14       | 0.11          |
| (1,1722) | 1:4:A:LEU:HD21  | 1:5:A:GLU:HA    | 14       | 0.11          |
| (1,1722) | 1:4:A:LEU:HD22  | 1:5:A:GLU:HA    | 14       | 0.11          |
| (1,1722) | 1:4:A:LEU:HD23  | 1:5:A:GLU:HA    | 14       | 0.11          |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG2   | 6        | 0.11          |
| (1,1698) | 1:1:A:MET:HG2   | 1:2:A:GLN:HG3   | 6        | 0.11          |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG2   | 6        | 0.11          |
| (1,1698) | 1:1:A:MET:HG3   | 1:2:A:GLN:HG3   | 6        | 0.11          |
| (1,1682) | 1:55:A:PHE:HE1  | 1:56:A:SER:HA   | 2        | 0.11          |
| (1,1682) | 1:55:A:PHE:HE2  | 1:56:A:SER:HA   | 2        | 0.11          |
| (1,1681) | 1:53:A:PHE:H    | 1:55:A:PHE:HD1  | 8        | 0.11          |
| (1,1681) | 1:53:A:PHE:H    | 1:55:A:PHE:HD2  | 8        | 0.11          |
| (1,1658) | 1:50:A:GLU:HB3  | 1:55:A:PHE:HD1  | 11       | 0.11          |
| (1,1658) | 1:50:A:GLU:HB3  | 1:55:A:PHE:HD2  | 11       | 0.11          |
| (1,1646) | 1:78:A:GLU:H    | 1:79:A:HIS:HD2  | 5        | 0.11          |
| (1,1388) | 1:24:A:LEU:HD11 | 1:25:A:THR:HA   | 1        | 0.11          |
| (1,1388) | 1:24:A:LEU:HD12 | 1:25:A:THR:HA   | 1        | 0.11          |
| (1,1388) | 1:24:A:LEU:HD13 | 1:25:A:THR:HA   | 1        | 0.11          |
| (1,1270) | 1:55:A:PHE:HD1  | 1:81:A:LEU:HD11 | 20       | 0.11          |
| (1,1270) | 1:55:A:PHE:HD1  | 1:81:A:LEU:HD12 | 20       | 0.11          |
| (1,1270) | 1:55:A:PHE:HD1  | 1:81:A:LEU:HD13 | 20       | 0.11          |
| (1,1270) | 1:55:A:PHE:HD2  | 1:81:A:LEU:HD11 | 20       | 0.11          |
| (1,1270) | 1:55:A:PHE:HD2  | 1:81:A:LEU:HD12 | 20       | 0.11          |
| (1,1270) | 1:55:A:PHE:HD2  | 1:81:A:LEU:HD13 | 20       | 0.11          |
| (1,1234) | 1:79:A:HIS:HA   | 1:82:A:SER:HB3  | 12       | 0.11          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD11 | 15       | 0.11          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD12 | 15       | 0.11          |
| (1,1120) | 1:57:A:VAL:HG11 | 1:62:A:ILE:HD13 | 15       | 0.11          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD11 | 15       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD12 | 15       | 0.11          |
| (1,1120) | 1:57:A:VAL:HG12 | 1:62:A:ILE:HD13 | 15       | 0.11          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD11 | 15       | 0.11          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD12 | 15       | 0.11          |
| (1,1120) | 1:57:A:VAL:HG13 | 1:62:A:ILE:HD13 | 15       | 0.11          |
| (1,1021) | 1:45:A:VAL:HB   | 1:46:A:ILE:HG13 | 18       | 0.11          |
| (1,1019) | 1:9:A:ASN:HD21  | 1:10:A:ILE:HA   | 15       | 0.11          |
| (1,964)  | 2:84:A:PNS:H282 | 1:40:A:MET:HG2  | 5        | 0.11          |
| (1,964)  | 2:84:A:PNS:H282 | 1:40:A:MET:HG3  | 5        | 0.11          |
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 11       | 0.11          |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 11       | 0.11          |
| (1,933)  | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3  | 11       | 0.11          |
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 15       | 0.11          |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 15       | 0.11          |
| (1,933)  | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3  | 15       | 0.11          |
| (1,916)  | 1:31:A:LEU:HG   | 1:67:A:PHE:H    | 14       | 0.11          |
| (1,874)  | 1:25:A:THR:HG21 | 1:28:A:SER:HB2  | 7        | 0.11          |
| (1,874)  | 1:25:A:THR:HG21 | 1:28:A:SER:HB3  | 7        | 0.11          |
| (1,874)  | 1:25:A:THR:HG22 | 1:28:A:SER:HB2  | 7        | 0.11          |
| (1,874)  | 1:25:A:THR:HG22 | 1:28:A:SER:HB3  | 7        | 0.11          |
| (1,874)  | 1:25:A:THR:HG23 | 1:28:A:SER:HB2  | 7        | 0.11          |
| (1,874)  | 1:25:A:THR:HG23 | 1:28:A:SER:HB3  | 7        | 0.11          |
| (1,833)  | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 1        | 0.11          |
| (1,833)  | 1:12:A:GLY:H    | 1:21:A:LYS:HG2  | 16       | 0.11          |
| (1,772)  | 1:10:A:ILE:HG21 | 1:13:A:ASP:HB2  | 2        | 0.11          |
| (1,772)  | 1:10:A:ILE:HG22 | 1:13:A:ASP:HB2  | 2        | 0.11          |
| (1,772)  | 1:10:A:ILE:HG23 | 1:13:A:ASP:HB2  | 2        | 0.11          |
| (1,772)  | 1:10:A:ILE:HG21 | 1:13:A:ASP:HB2  | 14       | 0.11          |
| (1,772)  | 1:10:A:ILE:HG22 | 1:13:A:ASP:HB2  | 14       | 0.11          |
| (1,772)  | 1:10:A:ILE:HG23 | 1:13:A:ASP:HB2  | 14       | 0.11          |
| (1,772)  | 1:10:A:ILE:HG21 | 1:13:A:ASP:HB2  | 18       | 0.11          |
| (1,772)  | 1:10:A:ILE:HG22 | 1:13:A:ASP:HB2  | 18       | 0.11          |
| (1,772)  | 1:10:A:ILE:HG23 | 1:13:A:ASP:HB2  | 18       | 0.11          |
| (1,741)  | 1:8:A:ARG:HG3   | 1:9:A:ASN:HA    | 8        | 0.11          |
| (1,730)  | 1:6:A:ALA:HB1   | 1:7:A:VAL:HG21  | 18       | 0.11          |
| (1,730)  | 1:6:A:ALA:HB1   | 1:7:A:VAL:HG22  | 18       | 0.11          |
| (1,730)  | 1:6:A:ALA:HB1   | 1:7:A:VAL:HG23  | 18       | 0.11          |
| (1,730)  | 1:6:A:ALA:HB2   | 1:7:A:VAL:HG21  | 18       | 0.11          |
| (1,730)  | 1:6:A:ALA:HB2   | 1:7:A:VAL:HG22  | 18       | 0.11          |
| (1,730)  | 1:6:A:ALA:HB2   | 1:7:A:VAL:HG23  | 18       | 0.11          |
| (1,730)  | 1:6:A:ALA:HB3   | 1:7:A:VAL:HG21  | 18       | 0.11          |
| (1,730)  | 1:6:A:ALA:HB3   | 1:7:A:VAL:HG22  | 18       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,730) | 1:6:A:ALA:HB3   | 1:7:A:VAL:HG23  | 18       | 0.11          |
| (1,668) | 1:29:A:VAL:HG21 | 1:33:A:ASN:HD21 | 6        | 0.11          |
| (1,668) | 1:29:A:VAL:HG22 | 1:33:A:ASN:HD21 | 6        | 0.11          |
| (1,668) | 1:29:A:VAL:HG23 | 1:33:A:ASN:HD21 | 6        | 0.11          |
| (1,649) | 1:6:A:ALA:HB1   | 1:9:A:ASN:HD22  | 8        | 0.11          |
| (1,649) | 1:6:A:ALA:HB2   | 1:9:A:ASN:HD22  | 8        | 0.11          |
| (1,649) | 1:6:A:ALA:HB3   | 1:9:A:ASN:HD22  | 8        | 0.11          |
| (1,649) | 1:6:A:ALA:HB1   | 1:9:A:ASN:HD22  | 13       | 0.11          |
| (1,649) | 1:6:A:ALA:HB2   | 1:9:A:ASN:HD22  | 13       | 0.11          |
| (1,649) | 1:6:A:ALA:HB3   | 1:9:A:ASN:HD22  | 13       | 0.11          |
| (1,649) | 1:6:A:ALA:HB1   | 1:9:A:ASN:HD22  | 16       | 0.11          |
| (1,649) | 1:6:A:ALA:HB2   | 1:9:A:ASN:HD22  | 16       | 0.11          |
| (1,649) | 1:6:A:ALA:HB3   | 1:9:A:ASN:HD22  | 16       | 0.11          |
| (1,643) | 1:2:A:GLN:HA    | 1:2:A:GLN:HE22  | 20       | 0.11          |
| (1,488) | 1:38:A:ASP:H    | 1:41:A:ALA:HB1  | 1        | 0.11          |
| (1,488) | 1:38:A:ASP:H    | 1:41:A:ALA:HB2  | 1        | 0.11          |
| (1,488) | 1:38:A:ASP:H    | 1:41:A:ALA:HB3  | 1        | 0.11          |
| (1,299) | 1:13:A:ASP:HA   | 1:15:A:LEU:H    | 1        | 0.11          |
| (1,299) | 1:13:A:ASP:HA   | 1:15:A:LEU:H    | 17       | 0.11          |
| (1,256) | 1:1:A:MET:HG3   | 1:4:A:LEU:H     | 12       | 0.11          |
| (1,185) | 1:4:A:LEU:H     | 1:7:A:VAL:HB    | 12       | 0.11          |
| (1,181) | 1:2:A:GLN:HA    | 1:5:A:GLU:H     | 7        | 0.11          |
| (1,164) | 1:30:A:LEU:H    | 1:69:A:THR:HB   | 10       | 0.11          |
| (1,44)  | 1:40:A:MET:HB3  | 1:43:A:VAL:H    | 9        | 0.11          |
| (1,13)  | 1:19:A:GLU:HG2  | 1:22:A:HIS:H    | 15       | 0.11          |
| (1,13)  | 1:19:A:GLU:HG3  | 1:22:A:HIS:H    | 15       | 0.11          |
| (1,12)  | 1:2:A:GLN:H     | 1:5:A:GLU:H     | 2        | 0.11          |
| (2,93)  | 1:67:A:PHE:H    | 1:64:A:ALA:O    | 9        | 0.1           |
| (2,91)  | 1:66:A:THR:H    | 1:63:A:SER:O    | 14       | 0.1           |
| (2,91)  | 1:66:A:THR:H    | 1:63:A:SER:O    | 20       | 0.1           |
| (2,81)  | 1:13:A:ASP:H    | 1:9:A:ASN:O     | 15       | 0.1           |
| (2,81)  | 1:13:A:ASP:H    | 1:9:A:ASN:O     | 19       | 0.1           |
| (2,77)  | 1:43:A:VAL:H    | 1:39:A:SER:O    | 3        | 0.1           |
| (2,77)  | 1:43:A:VAL:H    | 1:39:A:SER:O    | 6        | 0.1           |
| (2,75)  | 1:80:A:LYS:H    | 1:76:A:PHE:O    | 6        | 0.1           |
| (2,73)  | 1:79:A:HIS:H    | 1:75:A:LEU:O    | 9        | 0.1           |
| (2,73)  | 1:79:A:HIS:H    | 1:75:A:LEU:O    | 12       | 0.1           |
| (2,73)  | 1:79:A:HIS:H    | 1:75:A:LEU:O    | 19       | 0.1           |
| (2,67)  | 1:76:A:PHE:H    | 1:72:A:SER:O    | 17       | 0.1           |
| (2,62)  | 1:73:A:LEU:N    | 1:69:A:THR:O    | 7        | 0.1           |
| (2,61)  | 1:73:A:LEU:H    | 1:69:A:THR:O    | 6        | 0.1           |
| (2,61)  | 1:73:A:LEU:H    | 1:69:A:THR:O    | 10       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,61)   | 1:73:A:LEU:H    | 1:69:A:THR:O    | 12       | 0.1           |
| (2,61)   | 1:73:A:LEU:H    | 1:69:A:THR:O    | 15       | 0.1           |
| (2,57)   | 1:53:A:PHE:H    | 1:49:A:LEU:O    | 20       | 0.1           |
| (2,33)   | 1:9:A:ASN:H     | 1:5:A:GLU:O     | 8        | 0.1           |
| (2,28)   | 1:76:A:PHE:O    | 1:80:A:LYS:N    | 2        | 0.1           |
| (2,28)   | 1:76:A:PHE:O    | 1:80:A:LYS:N    | 4        | 0.1           |
| (2,21)   | 1:50:A:GLU:O    | 1:54:A:ASP:N    | 13       | 0.1           |
| (2,21)   | 1:50:A:GLU:O    | 1:54:A:ASP:N    | 17       | 0.1           |
| (2,2)    | 1:3:A:HIS:O     | 1:7:A:VAL:N     | 8        | 0.1           |
| (2,2)    | 1:3:A:HIS:O     | 1:7:A:VAL:N     | 20       | 0.1           |
| (2,1)    | 1:3:A:HIS:O     | 1:7:A:VAL:H     | 1        | 0.1           |
| (2,1)    | 1:3:A:HIS:O     | 1:7:A:VAL:H     | 2        | 0.1           |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 18       | 0.1           |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 18       | 0.1           |
| (1,2007) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 18       | 0.1           |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 18       | 0.1           |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 18       | 0.1           |
| (1,2007) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 18       | 0.1           |
| (1,1994) | 2:84:A:PNS:H371 | 1:46:A:ILE:HD11 | 10       | 0.1           |
| (1,1994) | 2:84:A:PNS:H371 | 1:46:A:ILE:HD12 | 10       | 0.1           |
| (1,1994) | 2:84:A:PNS:H371 | 1:46:A:ILE:HD13 | 10       | 0.1           |
| (1,1994) | 2:84:A:PNS:H372 | 1:46:A:ILE:HD11 | 10       | 0.1           |
| (1,1994) | 2:84:A:PNS:H372 | 1:46:A:ILE:HD12 | 10       | 0.1           |
| (1,1994) | 2:84:A:PNS:H372 | 1:46:A:ILE:HD13 | 10       | 0.1           |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD11 | 18       | 0.1           |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD12 | 18       | 0.1           |
| (1,1989) | 2:84:A:PNS:H431 | 1:62:A:ILE:HD13 | 18       | 0.1           |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD11 | 18       | 0.1           |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD12 | 18       | 0.1           |
| (1,1989) | 2:84:A:PNS:H432 | 1:62:A:ILE:HD13 | 18       | 0.1           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD11 | 15       | 0.1           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD12 | 15       | 0.1           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD13 | 15       | 0.1           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD21 | 15       | 0.1           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD22 | 15       | 0.1           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD23 | 15       | 0.1           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD11 | 19       | 0.1           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD12 | 19       | 0.1           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD13 | 19       | 0.1           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD21 | 19       | 0.1           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD22 | 19       | 0.1           |
| (1,1921) | 1:32:A:GLY:H    | 1:37:A:LEU:HD23 | 19       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1892) | 1:30:A:LEU:HD11 | 1:68:A:GLU:H    | 5        | 0.1           |
| (1,1892) | 1:30:A:LEU:HD12 | 1:68:A:GLU:H    | 5        | 0.1           |
| (1,1892) | 1:30:A:LEU:HD13 | 1:68:A:GLU:H    | 5        | 0.1           |
| (1,1892) | 1:30:A:LEU:HD21 | 1:68:A:GLU:H    | 5        | 0.1           |
| (1,1892) | 1:30:A:LEU:HD22 | 1:68:A:GLU:H    | 5        | 0.1           |
| (1,1892) | 1:30:A:LEU:HD23 | 1:68:A:GLU:H    | 5        | 0.1           |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 6        | 0.1           |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 6        | 0.1           |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 6        | 0.1           |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 6        | 0.1           |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 6        | 0.1           |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 6        | 0.1           |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD11 | 13       | 0.1           |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD12 | 13       | 0.1           |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD13 | 13       | 0.1           |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD21 | 13       | 0.1           |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD22 | 13       | 0.1           |
| (1,1859) | 1:24:A:LEU:HB3  | 1:70:A:LEU:HD23 | 13       | 0.1           |
| (1,1600) | 1:49:A:LEU:HD11 | 1:52:A:TYR:HD1  | 3        | 0.1           |
| (1,1600) | 1:49:A:LEU:HD11 | 1:52:A:TYR:HD2  | 3        | 0.1           |
| (1,1600) | 1:49:A:LEU:HD12 | 1:52:A:TYR:HD1  | 3        | 0.1           |
| (1,1600) | 1:49:A:LEU:HD12 | 1:52:A:TYR:HD2  | 3        | 0.1           |
| (1,1600) | 1:49:A:LEU:HD13 | 1:52:A:TYR:HD1  | 3        | 0.1           |
| (1,1600) | 1:49:A:LEU:HD13 | 1:52:A:TYR:HD2  | 3        | 0.1           |
| (1,1600) | 1:49:A:LEU:HD11 | 1:52:A:TYR:HD1  | 12       | 0.1           |
| (1,1600) | 1:49:A:LEU:HD11 | 1:52:A:TYR:HD2  | 12       | 0.1           |
| (1,1600) | 1:49:A:LEU:HD12 | 1:52:A:TYR:HD1  | 12       | 0.1           |
| (1,1600) | 1:49:A:LEU:HD12 | 1:52:A:TYR:HD2  | 12       | 0.1           |
| (1,1600) | 1:49:A:LEU:HD13 | 1:52:A:TYR:HD1  | 12       | 0.1           |
| (1,1600) | 1:49:A:LEU:HD13 | 1:52:A:TYR:HD2  | 12       | 0.1           |
| (1,1548) | 1:67:A:PHE:HA   | 1:73:A:LEU:HD21 | 19       | 0.1           |
| (1,1548) | 1:67:A:PHE:HA   | 1:73:A:LEU:HD22 | 19       | 0.1           |
| (1,1548) | 1:67:A:PHE:HA   | 1:73:A:LEU:HD23 | 19       | 0.1           |
| (1,1208) | 1:57:A:VAL:HG21 | 1:77:A:VAL:HA   | 5        | 0.1           |
| (1,1208) | 1:57:A:VAL:HG22 | 1:77:A:VAL:HA   | 5        | 0.1           |
| (1,1208) | 1:57:A:VAL:HG23 | 1:77:A:VAL:HA   | 5        | 0.1           |
| (1,1092) | 1:55:A:PHE:HE1  | 1:57:A:VAL:HB   | 11       | 0.1           |
| (1,1092) | 1:55:A:PHE:HE2  | 1:57:A:VAL:HB   | 11       | 0.1           |
| (1,1048) | 1:44:A:ASN:HB3  | 1:48:A:ALA:HB1  | 19       | 0.1           |
| (1,1048) | 1:44:A:ASN:HB3  | 1:48:A:ALA:HB2  | 19       | 0.1           |
| (1,1048) | 1:44:A:ASN:HB3  | 1:48:A:ALA:HB3  | 19       | 0.1           |
| (1,1021) | 1:45:A:VAL:HB   | 1:46:A:ILE:HG13 | 12       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1019) | 1:9:A:ASN:HD21  | 1:10:A:ILE:HA   | 16       | 0.1           |
| (1,967)  | 1:40:A:MET:HB3  | 1:42:A:VAL:HG21 | 7        | 0.1           |
| (1,967)  | 1:40:A:MET:HB3  | 1:42:A:VAL:HG22 | 7        | 0.1           |
| (1,967)  | 1:40:A:MET:HB3  | 1:42:A:VAL:HG23 | 7        | 0.1           |
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 6        | 0.1           |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 6        | 0.1           |
| (1,933)  | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3  | 6        | 0.1           |
| (1,933)  | 1:34:A:ILE:HG21 | 1:35:A:PRO:HD3  | 18       | 0.1           |
| (1,933)  | 1:34:A:ILE:HG22 | 1:35:A:PRO:HD3  | 18       | 0.1           |
| (1,933)  | 1:34:A:ILE:HG23 | 1:35:A:PRO:HD3  | 18       | 0.1           |
| (1,772)  | 1:10:A:ILE:HG21 | 1:13:A:ASP:HB2  | 13       | 0.1           |
| (1,772)  | 1:10:A:ILE:HG22 | 1:13:A:ASP:HB2  | 13       | 0.1           |
| (1,772)  | 1:10:A:ILE:HG23 | 1:13:A:ASP:HB2  | 13       | 0.1           |
| (1,755)  | 1:6:A:ALA:HB1   | 1:10:A:ILE:HD11 | 11       | 0.1           |
| (1,755)  | 1:6:A:ALA:HB1   | 1:10:A:ILE:HD12 | 11       | 0.1           |
| (1,755)  | 1:6:A:ALA:HB1   | 1:10:A:ILE:HD13 | 11       | 0.1           |
| (1,755)  | 1:6:A:ALA:HB2   | 1:10:A:ILE:HD11 | 11       | 0.1           |
| (1,755)  | 1:6:A:ALA:HB2   | 1:10:A:ILE:HD12 | 11       | 0.1           |
| (1,755)  | 1:6:A:ALA:HB2   | 1:10:A:ILE:HD13 | 11       | 0.1           |
| (1,755)  | 1:6:A:ALA:HB3   | 1:10:A:ILE:HD11 | 11       | 0.1           |
| (1,755)  | 1:6:A:ALA:HB3   | 1:10:A:ILE:HD12 | 11       | 0.1           |
| (1,755)  | 1:6:A:ALA:HB3   | 1:10:A:ILE:HD13 | 11       | 0.1           |
| (1,674)  | 1:64:A:ALA:HA   | 1:65:A:GLN:HE22 | 11       | 0.1           |
| (1,649)  | 1:6:A:ALA:HB1   | 1:9:A:ASN:HD22  | 17       | 0.1           |
| (1,649)  | 1:6:A:ALA:HB2   | 1:9:A:ASN:HD22  | 17       | 0.1           |
| (1,649)  | 1:6:A:ALA:HB3   | 1:9:A:ASN:HD22  | 17       | 0.1           |
| (1,439)  | 1:31:A:LEU:H    | 1:31:A:LEU:HB3  | 2        | 0.1           |
| (1,439)  | 1:31:A:LEU:H    | 1:31:A:LEU:HB3  | 3        | 0.1           |
| (1,400)  | 1:5:A:GLU:HG2   | 1:6:A:ALA:H     | 10       | 0.1           |
| (1,400)  | 1:5:A:GLU:HG3   | 1:6:A:ALA:H     | 10       | 0.1           |
| (1,383)  | 2:84:A:PNS:H311 | 2:84:A:PNS:H36  | 4        | 0.1           |
| (1,383)  | 2:84:A:PNS:H312 | 2:84:A:PNS:H36  | 4        | 0.1           |
| (1,383)  | 2:84:A:PNS:H313 | 2:84:A:PNS:H36  | 4        | 0.1           |
| (1,299)  | 1:13:A:ASP:HA   | 1:15:A:LEU:H    | 18       | 0.1           |
| (1,256)  | 1:1:A:MET:HG3   | 1:4:A:LEU:H     | 18       | 0.1           |
| (1,164)  | 1:30:A:LEU:H    | 1:69:A:THR:HB   | 13       | 0.1           |
| (1,146)  | 1:7:A:VAL:HG21  | 1:73:A:LEU:H    | 8        | 0.1           |
| (1,146)  | 1:7:A:VAL:HG22  | 1:73:A:LEU:H    | 8        | 0.1           |
| (1,146)  | 1:7:A:VAL:HG23  | 1:73:A:LEU:H    | 8        | 0.1           |
| (1,106)  | 1:80:A:LYS:HD2  | 1:81:A:LEU:H    | 9        | 0.1           |
| (1,106)  | 1:80:A:LYS:HD2  | 1:81:A:LEU:H    | 15       | 0.1           |
| (1,45)   | 2:84:A:PNS:H281 | 1:40:A:MET:H    | 18       | 0.1           |

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| Key    | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|--------|----------------|----------------|----------|---------------|
| (1,44) | 1:40:A:MET:HB3 | 1:43:A:VAL:H   | 11       | 0.1           |
| (1,44) | 1:40:A:MET:HB3 | 1:43:A:VAL:H   | 14       | 0.1           |
| (1,41) | 1:1:A:MET:HG2  | 1:4:A:LEU:H    | 14       | 0.1           |
| (1,38) | 1:79:A:HIS:H   | 1:80:A:LYS:HD3 | 15       | 0.1           |
| (1,13) | 1:19:A:GLU:HG2 | 1:22:A:HIS:H   | 8        | 0.1           |
| (1,13) | 1:19:A:GLU:HG3 | 1:22:A:HIS:H   | 8        | 0.1           |
| (1,12) | 1:2:A:GLN:H    | 1:5:A:GLU:H    | 11       | 0.1           |

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

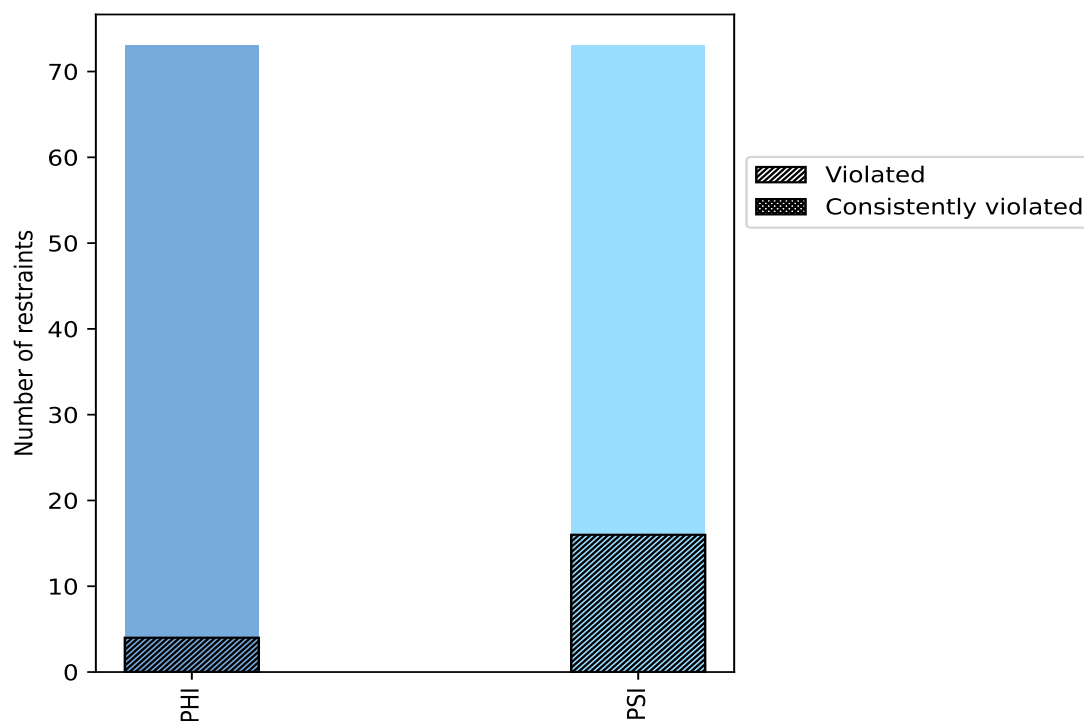
### 10.1 Summary of dihedral-angle violations [i](#)

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        | 73    | 50.0           | 4                     | 5.5            | 2.7            | 0                                  | 0.0            | 0.0            |
| PSI        | 73    | 50.0           | 16                    | 21.9           | 11.0           | 0                                  | 0.0            | 0.0            |
| Total      | 146   | 100.0          | 20                    | 13.7           | 13.7           | 0                                  | 0.0            | 0.0            |

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

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



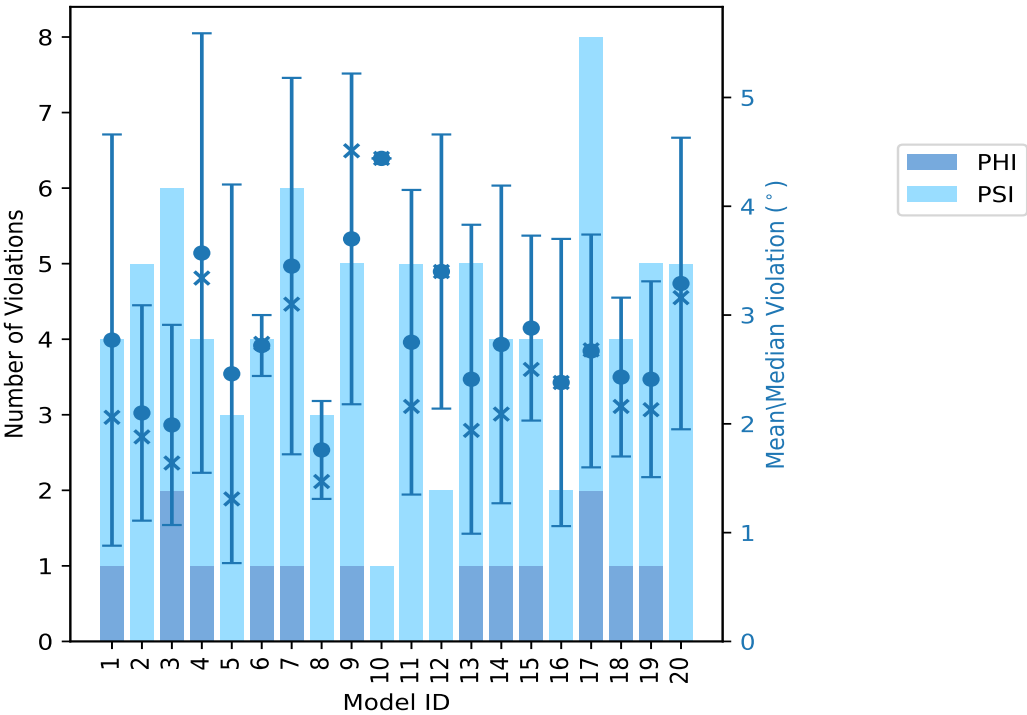
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 1                    | 3   | 4     | 2.77     | 5.92    | 1.89   | 2.06       |
| 2        | 0                    | 5   | 5     | 2.1      | 3.45    | 0.99   | 1.88       |
| 3        | 2                    | 4   | 6     | 1.99     | 3.32    | 0.92   | 1.64       |
| 4        | 1                    | 3   | 4     | 3.57     | 6.19    | 2.02   | 3.34       |
| 5        | 0                    | 3   | 3     | 2.46     | 4.92    | 1.74   | 1.31       |
| 6        | 1                    | 3   | 4     | 2.72     | 3.01    | 0.28   | 2.74       |
| 7        | 1                    | 5   | 6     | 3.45     | 5.73    | 1.73   | 3.1        |
| 8        | 0                    | 3   | 3     | 1.76     | 2.39    | 0.45   | 1.47       |
| 9        | 1                    | 4   | 5     | 3.7      | 5.2     | 1.52   | 4.51       |
| 10       | 0                    | 1   | 1     | 4.44     | 4.44    | 0.0    | 4.44       |
| 11       | 0                    | 5   | 5     | 2.75     | 5.46    | 1.4    | 2.16       |
| 12       | 0                    | 2   | 2     | 3.4      | 4.67    | 1.26   | 3.4        |
| 13       | 1                    | 4   | 5     | 2.41     | 4.92    | 1.42   | 1.94       |
| 14       | 1                    | 3   | 4     | 2.73     | 5.22    | 1.46   | 2.09       |
| 15       | 1                    | 3   | 4     | 2.88     | 4.33    | 0.85   | 2.5        |
| 16       | 0                    | 2   | 2     | 2.38     | 3.69    | 1.32   | 2.38       |
| 17       | 2                    | 6   | 8     | 2.67     | 4.57    | 1.07   | 2.68       |
| 18       | 1                    | 3   | 4     | 2.43     | 3.64    | 0.73   | 2.16       |
| 19       | 1                    | 4   | 5     | 2.41     | 3.69    | 0.9    | 2.13       |
| 20       | 0                    | 5   | 5     | 3.29     | 5.49    | 1.34   | 3.16       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

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

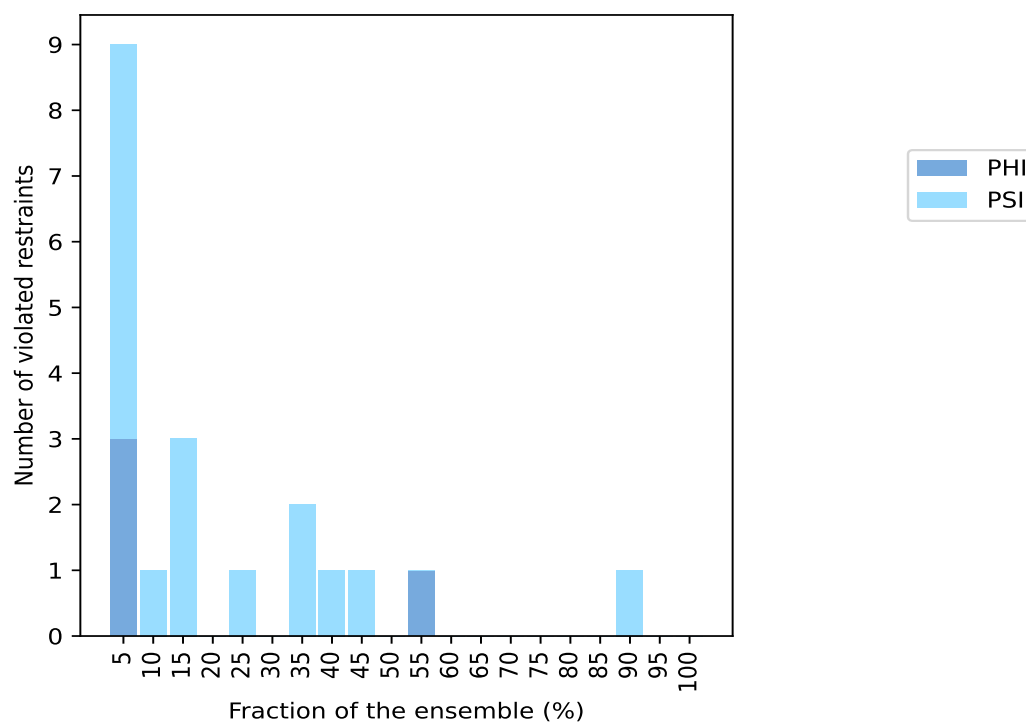
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |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

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

### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

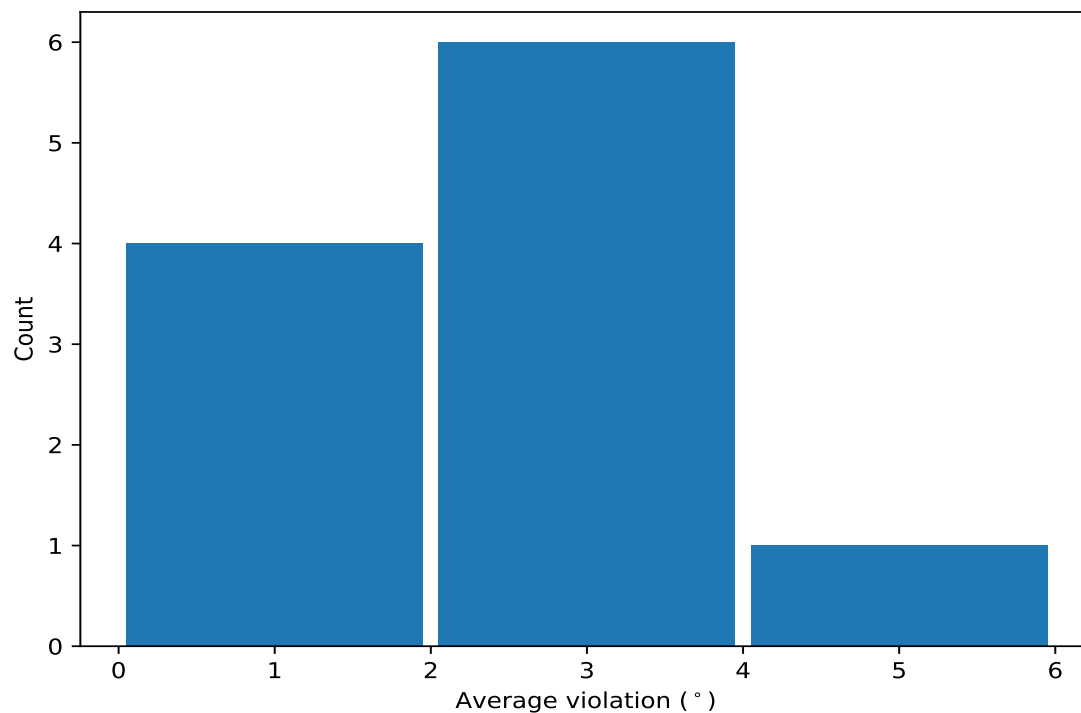


## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



#### 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.

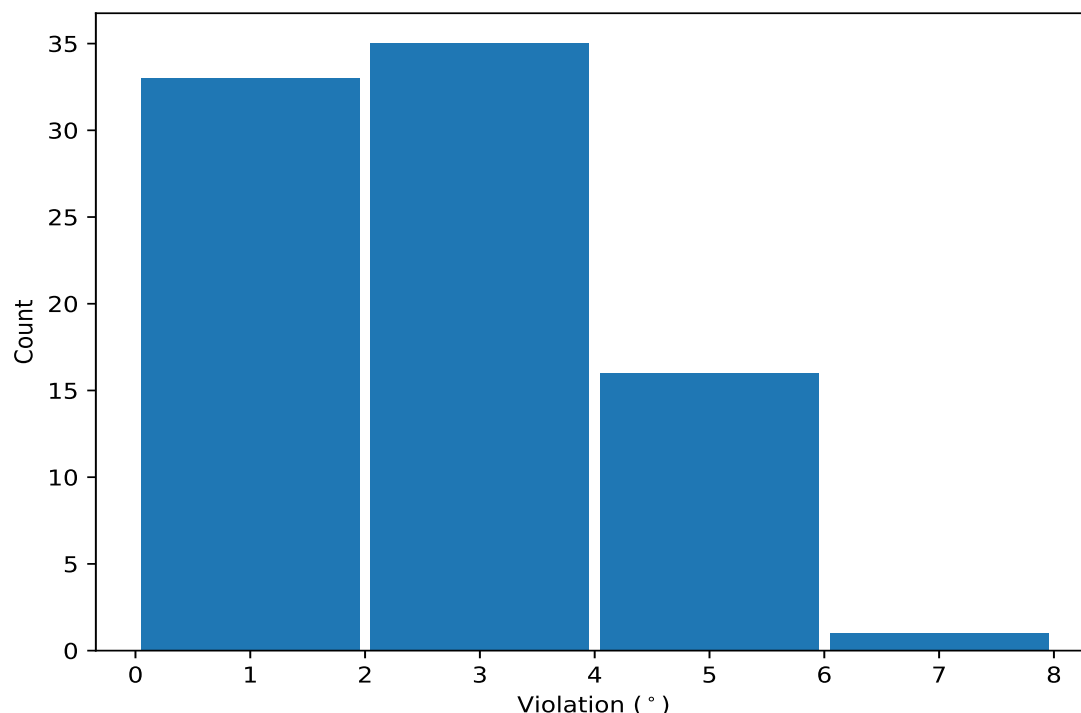
| Key     | Atom-1       | Atom-2        | Atom-3       | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|--------------|--------------|---------------------|------|-----------------|--------|
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C | 1:78:A:GLU:N | 18                  | 4.29 | 1.12            | 4.47   |
| (1,1)   | 1:1:A:MET:C  | 1:2:A:GLN:N   | 1:2:A:GLN:CA | 1:2:A:GLN:C  | 11                  | 2.9  | 1.17            | 2.92   |
| (1,14)  | 1:8:A:ARG:N  | 1:8:A:ARG:CA  | 1:8:A:ARG:C  | 1:9:A:ASN:N  | 9                   | 2.51 | 1.22            | 2.21   |
| (1,64)  | 1:39:A:SER:N | 1:39:A:SER:CA | 1:39:A:SER:C | 1:40:A:MET:N | 8                   | 3.46 | 1.23            | 3.0    |
| (1,52)  | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:GLY:N | 7                   | 2.16 | 0.72            | 2.06   |
| (1,22)  | 1:12:A:GLY:N | 1:12:A:GLY:CA | 1:12:A:GLY:C | 1:13:A:ASP:N | 7                   | 1.49 | 0.37            | 1.42   |
| (1,144) | 1:81:A:LEU:N | 1:81:A:LEU:CA | 1:81:A:LEU:C | 1:82:A:SER:N | 5                   | 1.76 | 0.81            | 1.3    |
| (1,30)  | 1:16:A:ASN:N | 1:16:A:ASN:CA | 1:16:A:ASN:C | 1:17:A:LEU:N | 3                   | 2.11 | 0.67            | 1.87   |
| (1,98)  | 1:56:A:SER:N | 1:56:A:SER:CA | 1:56:A:SER:C | 1:57:A:VAL:N | 3                   | 1.76 | 0.57            | 1.88   |
| (1,138) | 1:78:A:GLU:N | 1:78:A:GLU:CA | 1:78:A:GLU:C | 1:79:A:HIS:N | 3                   | 1.51 | 0.48            | 1.31   |
| (1,116) | 1:65:A:GLN:N | 1:65:A:GLN:CA | 1:65:A:GLN:C | 1:66:A:THR:N | 2                   | 2.1  | 0.87            | 2.1    |

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

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

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

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



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

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

| Key     | Atom-1       | Atom-2        | Atom-3       | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|--------------|--------------|----------|---------------|
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C | 1:78:A:GLU:N | 4        | 6.19          |
| (1,64)  | 1:39:A:SER:N | 1:39:A:SER:CA | 1:39:A:SER:C | 1:40:A:MET:N | 1        | 5.92          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C | 1:78:A:GLU:N | 7        | 5.73          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C | 1:78:A:GLU:N | 20       | 5.49          |
| (1,100) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:ASP:N | 7        | 5.47          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C | 1:78:A:GLU:N | 11       | 5.46          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C | 1:78:A:GLU:N | 14       | 5.22          |
| (1,1)   | 1:1:A:MET:C  | 1:2:A:GLN:N   | 1:2:A:GLN:CA | 1:2:A:GLN:C  | 9        | 5.2           |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C | 1:78:A:GLU:N | 5        | 4.92          |
| (1,14)  | 1:8:A:ARG:N  | 1:8:A:ARG:CA  | 1:8:A:ARG:C  | 1:9:A:ASN:N  | 13       | 4.92          |
| (1,1)   | 1:1:A:MET:C  | 1:2:A:GLN:N   | 1:2:A:GLN:CA | 1:2:A:GLN:C  | 4        | 4.89          |
| (1,64)  | 1:39:A:SER:N | 1:39:A:SER:CA | 1:39:A:SER:C | 1:40:A:MET:N | 9        | 4.7           |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C | 1:78:A:GLU:N | 12       | 4.67          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C | 1:78:A:GLU:N | 17       | 4.57          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C  | 1:78:A:GLU:N | 9        | 4.51          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C  | 1:78:A:GLU:N | 10       | 4.44          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C  | 1:78:A:GLU:N | 15       | 4.33          |
| (1,14)  | 1:8:A:ARG:N  | 1:8:A:ARG:CA  | 1:8:A:ARG:C   | 1:9:A:ASN:N  | 7        | 3.98          |
| (1,64)  | 1:39:A:SER:N | 1:39:A:SER:CA | 1:39:A:SER:C  | 1:40:A:MET:N | 20       | 3.93          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C  | 1:78:A:GLU:N | 16       | 3.69          |
| (1,52)  | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C  | 1:32:A:GLY:N | 19       | 3.69          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C  | 1:78:A:GLU:N | 18       | 3.64          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C  | 1:78:A:GLU:N | 2        | 3.45          |
| (1,64)  | 1:39:A:SER:N | 1:39:A:SER:CA | 1:39:A:SER:C  | 1:40:A:MET:N | 17       | 3.42          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C  | 1:78:A:GLU:N | 3        | 3.32          |
| (1,146) | 1:82:A:SER:N | 1:82:A:SER:CA | 1:82:A:SER:C  | 1:83:A:HIS:N | 17       | 3.28          |
| (1,144) | 1:81:A:LEU:N | 1:81:A:LEU:CA | 1:81:A:LEU:C  | 1:82:A:SER:N | 20       | 3.16          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C  | 1:78:A:GLU:N | 19       | 3.14          |
| (1,1)   | 1:1:A:MET:C  | 1:2:A:GLN:N   | 1:2:A:GLN:CA  | 1:2:A:GLN:C  | 17       | 3.14          |
| (1,1)   | 1:1:A:MET:C  | 1:2:A:GLN:N   | 1:2:A:GLN:CA  | 1:2:A:GLN:C  | 3        | 3.13          |
| (1,14)  | 1:8:A:ARG:N  | 1:8:A:ARG:CA  | 1:8:A:ARG:C   | 1:9:A:ASN:N  | 9        | 3.06          |
| (1,30)  | 1:16:A:ASN:N | 1:16:A:ASN:CA | 1:16:A:ASN:C  | 1:17:A:LEU:N | 2        | 3.02          |
| (1,1)   | 1:1:A:MET:C  | 1:2:A:GLN:N   | 1:2:A:GLN:CA  | 1:2:A:GLN:C  | 6        | 3.01          |
| (1,116) | 1:65:A:GLN:N | 1:65:A:GLN:CA | 1:65:A:GLN:C  | 1:66:A:THR:N | 6        | 2.97          |
| (1,1)   | 1:1:A:MET:C  | 1:2:A:GLN:N   | 1:2:A:GLN:CA  | 1:2:A:GLN:C  | 13       | 2.92          |
| (1,14)  | 1:8:A:ARG:N  | 1:8:A:ARG:CA  | 1:8:A:ARG:C   | 1:9:A:ASN:N  | 11       | 2.64          |
| (1,64)  | 1:39:A:SER:N | 1:39:A:SER:CA | 1:39:A:SER:C  | 1:40:A:MET:N | 15       | 2.58          |
| (1,52)  | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C  | 1:32:A:GLY:N | 1        | 2.52          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C  | 1:78:A:GLU:N | 6        | 2.51          |
| (1,1)   | 1:1:A:MET:C  | 1:2:A:GLN:N   | 1:2:A:GLN:CA  | 1:2:A:GLN:C  | 15       | 2.43          |
| (1,64)  | 1:39:A:SER:N | 1:39:A:SER:CA | 1:39:A:SER:C  | 1:40:A:MET:N | 18       | 2.4           |
| (1,64)  | 1:39:A:SER:N | 1:39:A:SER:CA | 1:39:A:SER:C  | 1:40:A:MET:N | 8        | 2.39          |
| (1,98)  | 1:56:A:SER:N | 1:56:A:SER:CA | 1:56:A:SER:C  | 1:57:A:VAL:N | 6        | 2.38          |
| (1,64)  | 1:39:A:SER:N | 1:39:A:SER:CA | 1:39:A:SER:C  | 1:40:A:MET:N | 14       | 2.3           |
| (1,42)  | 1:25:A:THR:N | 1:25:A:THR:CA | 1:25:A:THR:C  | 1:26:A:ALA:N | 7        | 2.22          |
| (1,14)  | 1:8:A:ARG:N  | 1:8:A:ARG:CA  | 1:8:A:ARG:C   | 1:9:A:ASN:N  | 17       | 2.21          |
| (1,138) | 1:78:A:GLU:N | 1:78:A:GLU:CA | 1:78:A:GLU:C  | 1:79:A:HIS:N | 15       | 2.18          |
| (1,145) | 1:81:A:LEU:C | 1:82:A:SER:N  | 1:82:A:SER:CA | 1:82:A:SER:C | 17       | 2.16          |
| (1,144) | 1:81:A:LEU:N | 1:81:A:LEU:CA | 1:81:A:LEU:C  | 1:82:A:SER:N | 11       | 2.16          |
| (1,52)  | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C  | 1:32:A:GLY:N | 12       | 2.14          |
| (1,1)   | 1:1:A:MET:C  | 1:2:A:GLN:N   | 1:2:A:GLN:CA  | 1:2:A:GLN:C  | 19       | 2.13          |
| (1,52)  | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C  | 1:32:A:GLY:N | 7        | 2.06          |
| (1,22)  | 1:12:A:GLY:N | 1:12:A:GLY:CA | 1:12:A:GLY:C  | 1:13:A:ASP:N | 20       | 1.98          |
| (1,14)  | 1:8:A:ARG:N  | 1:8:A:ARG:CA  | 1:8:A:ARG:C   | 1:9:A:ASN:N  | 3        | 1.98          |
| (1,136) | 1:77:A:VAL:N | 1:77:A:VAL:CA | 1:77:A:VAL:C  | 1:78:A:GLU:N | 13       | 1.94          |
| (1,22)  | 1:12:A:GLY:N | 1:12:A:GLY:CA | 1:12:A:GLY:C  | 1:13:A:ASP:N | 19       | 1.93          |
| (1,1)   | 1:1:A:MET:C  | 1:2:A:GLN:N   | 1:2:A:GLN:CA  | 1:2:A:GLN:C  | 18       | 1.92          |
| (1,126) | 1:72:A:SER:N | 1:72:A:SER:CA | 1:72:A:SER:C  | 1:73:A:LEU:N | 20       | 1.89          |
| (1,1)   | 1:1:A:MET:C  | 1:2:A:GLN:N   | 1:2:A:GLN:CA  | 1:2:A:GLN:C  | 14       | 1.89          |
| (1,98)  | 1:56:A:SER:N | 1:56:A:SER:CA | 1:56:A:SER:C  | 1:57:A:VAL:N | 2        | 1.88          |
| (1,30)  | 1:16:A:ASN:N | 1:16:A:ASN:CA | 1:16:A:ASN:C  | 1:17:A:LEU:N | 11       | 1.87          |
| (1,22)  | 1:12:A:GLY:N | 1:12:A:GLY:CA | 1:12:A:GLY:C  | 1:13:A:ASP:N | 4        | 1.78          |
| (1,52)  | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C  | 1:32:A:GLY:N | 18       | 1.77          |
| (1,52)  | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C  | 1:32:A:GLY:N | 11       | 1.63          |
| (1,139) | 1:78:A:GLU:C | 1:79:A:HIS:N  | 1:79:A:HIS:CA | 1:79:A:HIS:C | 1        | 1.59          |

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*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,14)  | 1:8:A:ARG:N  | 1:8:A:ARG:CA  | 1:8:A:ARG:C   | 1:9:A:ASN:N  | 14       | 1.52          |
| (1,26)  | 1:14:A:VAL:N | 1:14:A:VAL:CA | 1:14:A:VAL:C  | 1:15:A:LEU:N | 8        | 1.47          |
| (1,30)  | 1:16:A:ASN:N | 1:16:A:ASN:CA | 1:16:A:ASN:C  | 1:17:A:LEU:N | 4        | 1.43          |
| (1,22)  | 1:12:A:GLY:N | 1:12:A:GLY:CA | 1:12:A:GLY:C  | 1:13:A:ASP:N | 8        | 1.42          |
| (1,138) | 1:78:A:GLU:N | 1:78:A:GLU:CA | 1:78:A:GLU:C  | 1:79:A:HIS:N | 5        | 1.31          |
| (1,144) | 1:81:A:LEU:N | 1:81:A:LEU:CA | 1:81:A:LEU:C  | 1:82:A:SER:N | 17       | 1.3           |
| (1,52)  | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C  | 1:32:A:GLY:N | 3        | 1.29          |
| (1,22)  | 1:12:A:GLY:N | 1:12:A:GLY:CA | 1:12:A:GLY:C  | 1:13:A:ASP:N | 17       | 1.27          |
| (1,116) | 1:65:A:GLN:N | 1:65:A:GLN:CA | 1:65:A:GLN:C  | 1:66:A:THR:N | 13       | 1.23          |
| (1,1)   | 1:1:A:MET:C  | 1:2:A:GLN:N   | 1:2:A:GLN:CA  | 1:2:A:GLN:C  | 7        | 1.22          |
| (1,33)  | 1:18:A:GLY:C | 1:19:A:GLU:N  | 1:19:A:GLU:CA | 1:19:A:GLU:C | 3        | 1.17          |
| (1,14)  | 1:8:A:ARG:N  | 1:8:A:ARG:CA  | 1:8:A:ARG:C   | 1:9:A:ASN:N  | 19       | 1.17          |
| (1,144) | 1:81:A:LEU:N | 1:81:A:LEU:CA | 1:81:A:LEU:C  | 1:82:A:SER:N | 5        | 1.14          |
| (1,14)  | 1:8:A:ARG:N  | 1:8:A:ARG:CA  | 1:8:A:ARG:C   | 1:9:A:ASN:N  | 2        | 1.1           |
| (1,22)  | 1:12:A:GLY:N | 1:12:A:GLY:CA | 1:12:A:GLY:C  | 1:13:A:ASP:N | 16       | 1.06          |
| (1,138) | 1:78:A:GLU:N | 1:78:A:GLU:CA | 1:78:A:GLU:C  | 1:79:A:HIS:N | 1        | 1.05          |
| (1,24)  | 1:13:A:ASP:N | 1:13:A:ASP:CA | 1:13:A:ASP:C  | 1:14:A:VAL:N | 3        | 1.04          |
| (1,144) | 1:81:A:LEU:N | 1:81:A:LEU:CA | 1:81:A:LEU:C  | 1:82:A:SER:N | 2        | 1.03          |
| (1,22)  | 1:12:A:GLY:N | 1:12:A:GLY:CA | 1:12:A:GLY:C  | 1:13:A:ASP:N | 13       | 1.02          |
| (1,98)  | 1:56:A:SER:N | 1:56:A:SER:CA | 1:56:A:SER:C  | 1:57:A:VAL:N | 9        | 1.01          |